

Supplementary Information

Computational discovery and proof-of-concept synthesis of super-ordered quinary MAB phases (s-MAB) with combined in-plane and out-of-plane chemical ordering

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Table S1. PBE potential used for elements considered in this work.

Element	POTCAR	Valence electrons
Sc	Sc_sv	4s 3d 3p 3s
Y	Y_sv	5s 4d 4p 4s
Ti	Ti_pv	4s 3d 3p
Zr	Zr_sv	5s 4d 4p 4s
Hf	Hf_pv	6s 5d 5p
V	V_pv	4s 3d 3p
Nb	Nb_pv	5s 4d 4p
Ta	Ta_pv	6s 5d 5p
Cr	Cr_pv	4s 3d 3p
Mo	Mo_pv	5s 4d 4p
W	W_pv	6s 5d 5p
Mn	Mn_pv	4s 3d 3p
Fe	Fe_pv	4s 3d 3p
Al	Al	3p 3s
B	B	2p 2s

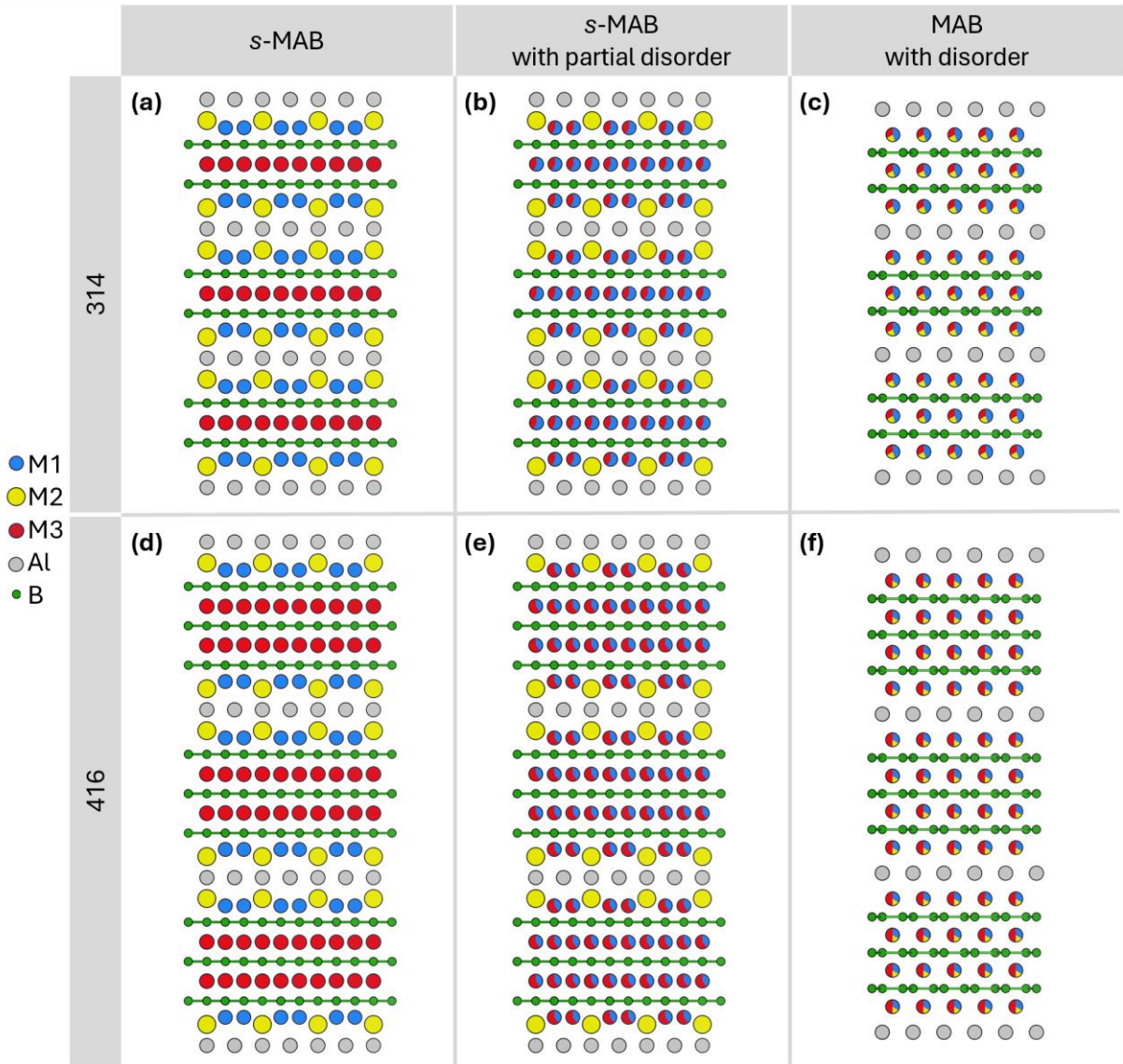


Figure S1. Different distribution of metals M1, M2, and M3 in 314 and 416 MAB phases. (a,d) s-MAB phase with combined in- and out-of-plane order with space group symmetry $P6/mmm$, (b,e) s-MAB phase with partial disorder where M2 are arranged orderly in-plane in the metal layer next to A while of M1 + M3 are disordered on the other metal sites with space group symmetry $P6/mmm$, and (c,f) complete disorder of M1, M2, and M3 across all metal layers in MAB phase with space group symmetry $P-6m2$.

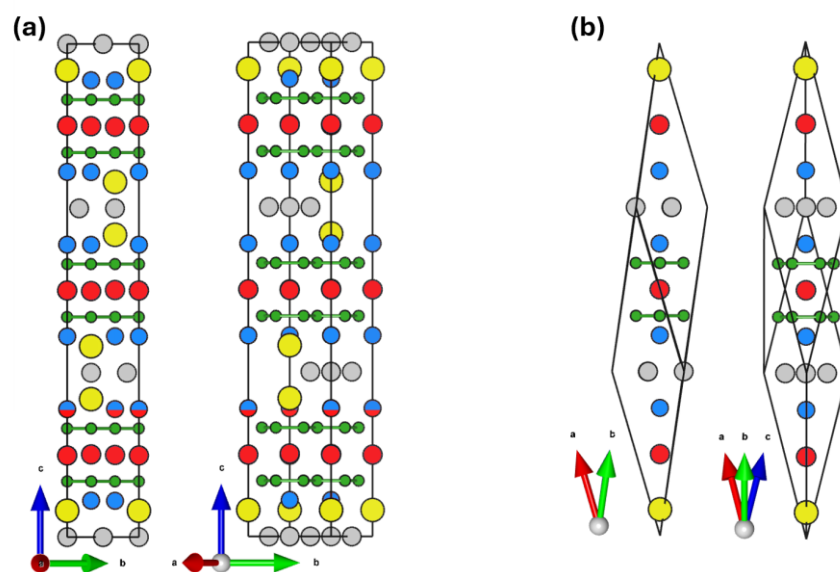


Figure S2. $M1_{4/3}M2_{2/3}M3AlB_4$ s-MAB structure of space group $R\bar{3}m$ (no. 166) in its (a) hexagonal and (b) rhombohedral unit cell representation.

Table S2. Calculated energy (E) and stability at 2000 K (ΔG_{cp}^{s-MAB} , $\Delta G_{cp}^{partial\ disorder}$, $\Delta G_{cp}^{disorder}$) for M2 = Sc in *s*-MAB, *s*-MAB with disorder, and MAB with disorder for 314 MAB phases along with corresponding energy for their competing phases and identified set of most competing phases. Phases modelled with solid solution disorder have a contribution from configurational entropy evaluated at 2000 K. Competing phases in bold highlight when a MAB phase is part of the set of most competing phases.

			Energy (eV/atom)					ΔG_{cp} (meV/atom)					Set of most competing phases	
M1	M2	M3	<i>s</i> -MAB (no. 191)	<i>s</i> -MAB (no. 194)	<i>s</i> -MAB (no. 166)	<i>s</i> -MAB disorder	MAB disorder	Competing phases	<i>s</i> -MAB (no. 191)	<i>s</i> -MAB (no. 194)	<i>s</i> -MAB (no. 166)	<i>s</i> -MAB partial disorder	MAB disorder	
Sc	Sc	Y	N/A	N/A	N/A	N/A	-6.868846	-6.934202	N/A	N/A	N/A	N/A	65	AlY ₂ + Al ₂ Y + ScB ₂
Sc	Sc	Ti	N/A	N/A	N/A	N/A	-7.190021	-7.217586	N/A	N/A	N/A	N/A	28	(Sc _{0.5} Ti _{0.5})B ₂ + AlSc
Sc	Sc	Zr	N/A	N/A	N/A	N/A	-7.260930	-7.290513	N/A	N/A	N/A	N/A	30	(Sc _{0.5} Zr _{0.5})B ₂ + AlSc
Sc	Sc	Hf	N/A	N/A	N/A	N/A	-7.446013	-7.484032	N/A	N/A	N/A	N/A	38	(Sc _{0.5} Hf _{0.5})B ₂ + AlSc
Sc	Sc	V	N/A	N/A	N/A	N/A	-7.273244	-7.301387	N/A	N/A	N/A	N/A	28	Al ₂ Sc + VB + ScB ₂
Sc	Sc	Nb	N/A	N/A	N/A	N/A	-7.449248	-7.455017	N/A	N/A	N/A	N/A	6	(Nb _{0.5} Sc _{0.5}) ₄ AlB ₆ + AlSc + (Sc _{0.75} Nb _{0.25})B ₂
Sc	Sc	Ta	N/A	N/A	N/A	N/A	-7.668477	-7.676209	N/A	N/A	N/A	N/A	8	(Ta _{0.5} Sc _{0.5}) ₄ AlB ₆ + AlSc + (Sc _{0.75} Ta _{0.25})B ₂
Y	Sc	Sc	-6.793402	-6.750182	-6.793840	-6.797728	-6.848917	-6.908148	115	158	114	110	59	(Sc _{0.75} Y _{0.25})B ₂ + AlY ₂ + Al ₂ Y + ScB ₂
Y	Sc	Y	-6.726773	-6.682536	-6.727291	N/A	-6.796384	-6.826152	99	144	99	N/A	30	(Sc _{0.75} Y _{0.25})B ₂ + (Y _{0.75} Sc _{0.25})B ₂ + AlY ₂ + Al ₂ Y
Y	Sc	Ti	-7.057420	-7.014816	-7.056898	-7.029792	-7.077685	-7.198439	141	184	142	169	121	(Ti _{0.5} Sc _{0.5})B ₂ + (Y _{0.75} Sc _{0.25})B ₂ + (Ti _{0.75} Sc _{0.25})B ₂ + AlY ₂ + Al ₂ Y
Y	Sc	Zr	-7.145898	-7.103549	-7.145184	-7.122631	-7.175981	-7.267925	122	164	123	145	92	(Y _{0.75} Zr _{0.25})B ₂ + (Zr _{0.75} Sc _{0.25})B ₂ + (Zr _{0.5} Sc _{0.5})B ₂ + AlY ₂ + Al ₂ Y
Y	Sc	Hf	-7.334600	-7.292382	-7.333939	-7.314495	-7.350956	-7.459213	125	167	125	145	108	(Hf _{0.5} Sc _{0.5})B ₂ + AlY ₂ + YB ₂ + Al ₂ Y + (Hf _{0.75} Sc _{0.25})B ₂
Y	Sc	V	-7.108138	-7.065041	-7.108556	-7.066479	-7.145238	-7.252925	145	188	144	186	108	ScY ₃ B ₈ + AlY ₂ + Al ₂ Y + VB + (Sc _{0.75} V _{0.25})B ₂
Y	Sc	Nb	-7.290470	-7.248949	-7.291109	-7.269494	-7.337188	-7.422376	132	169	126	148	80	(Nb _{0.5} Y _{0.5})B ₂ + AlY ₂ + Al ₂ Y + (Nb _{0.5} Sc _{0.5})B ₂
Y	Sc	Ta	-7.512276	-7.469945	-7.512888	-7.485725	-7.550988	-7.644786	133	167	124	151	86	AlY ₂ + (Y _{0.5} Ta _{0.5})B ₂ + Al ₂ Y + (Ta _{0.5} Sc _{0.5})B ₂
Y	Sc	Cr	-7.032743	-6.988255	-7.032966	N/A	N/A	-7.263264	231	275	230	N/A	N/A	AlY ₂ + CrYB ₄ + Al ₂ Y + CrB + ScB ₂
Y	Sc	Mo	-7.240554	-7.193286	-7.240581	N/A	N/A	-7.418677	178	225	178	N/A	N/A	MoYB ₄ + AlY ₂ + Al ₂ Y + Mo_{4/3}Y_{2/3}AlB₂ + (Sc _{0.75} Mo _{0.25})B ₂
Y	Sc	W	-7.464415	-7.415797	-7.464522	N/A	N/A	-7.658176	194	242	194	N/A	N/A	ScW ₂ B ₄ + (Sc _{0.75} W _{0.25})B ₂ + WY ₃ B ₇ + Al ₂ Y + W
Y	Sc	Mn	-6.957381	-6.912484	-6.957836	N/A	N/A	-7.197242	240	285	239	N/A	N/A	Mn_{4/3}Y_{2/3}AlB₂ + MnY ₃ B ₇ + AlY ₂ + Al ₂ Y + ScB ₂
Y	Sc	Fe	-6.807214	-6.763523	-6.807318	N/A	N/A	-7.094764	288	331	287	N/A	N/A	FeYB ₄ + FeY ₃ B ₇ + Fe ₂ YB ₂ + Al ₂ Y + ScB ₂
Ti	Sc	Sc	-7.238580	-7.238448	-7.238788	-7.265219	-7.273551	-7.311191	73	73	72	46	38	(Ti _{0.5} Sc _{0.5})B ₂ + AlSc + (Ti _{0.75} Sc _{0.25})B ₂
Ti	Sc	Y	-7.142570	-7.142188	-7.142489	-7.129043	-7.178423	-7.322119	180	180	180	193	144	(Ti _{0.5} Sc _{0.5})B ₂ + (Ti _{0.75} Sc _{0.25})B ₂ + AlY ₂ + Al ₂ Y
Ti	Sc	Ti	-7.520980	-7.521737	-7.521588	N/A	-7.541285	-7.549168	28	27	28	N/A	8	(Ti _{0.83} Sc _{0.17}) ₄ AlB ₆ + AlSc + AlTi
Ti	Sc	Zr	-7.574064	-7.574708	-7.574607	-7.578946	-7.588403	-7.618055	44	43	43	39	30	(Ti _{0.83} Sc _{0.17}) ₄ AlB ₆ + Al ₃ Zr ₂ + (Zr _{0.83} Sc _{0.17}) ₄ AlB ₆ + AlSc + Al ₃ Zr ₄
Ti	Sc	Hf	-7.765788	-7.766525	-7.766393	-7.774037	-7.778818	-7.800715	35	34	34	27	22	(Ti _{0.83} Sc _{0.17}) ₄ AlB ₆ + (Hf _{0.83} Sc _{0.17}) ₄ AlB ₆ + Al ₂ Sc + AlSc + Al ₃ Hf ₄
Ti	Sc	V	-7.582383	-7.581806	-7.581641	-7.641001	-7.621200	-7.676777	94	95	95	36	56	Al ₂ Sc + (Ti _{0.75} Sc _{0.25})B ₂ + VB + TiB ₂
Ti	Sc	Nb	-7.727638	-7.726563	-7.726332	-7.775927	-7.774580	-7.788686	61	62	62	13	14	(Nb _{0.75} Ti _{0.25})B + (Nb _{0.5} Sc _{0.5}) ₄ AlB ₆ + Al ₃ Nb + Al ₂ Sc + TiB ₂
Ti	Sc	Ta	-7.946838	-7.945559	-7.945423	-7.996299	-7.995913	-8.019878	73	74	74	24	24	(Ti _{0.75} Sc _{0.25})B ₂ + Al ₃ Sc + (Ta _{0.75} Ti _{0.25})B ₂
Ti	Sc	Cr	-7.506803	-7.506682	-7.506603	N/A	N/A	-7.671138	164	164	165	N/A	N/A	(Ti _{0.75} Sc _{0.25})B ₂ + Cr ₅ B ₃ + Al ₃ Sc + CrB + TiB ₂
Ti	Sc	Mo	-7.681685	-7.680042	-7.679846	N/A	N/A	-7.838242	157	158	158	N/A	N/A	Al ₂ Sc + (Ti _{0.75} Sc _{0.25})B ₂ + Al ₃ Mo ₃ + (Sc _{0.75} Mo _{0.25})B ₂ + AlMo ₃
Ti	Sc	W	-7.896646	-7.895110	-7.895040	N/A	N/A	-8.071012	174	176	176	N/A	N/A	(W _{0.75} Ti _{0.25})B ₂ + (Ti _{0.75} Sc _{0.25})B ₂ + Al ₃ Sc
Ti	Sc	Mn	-7.430143	-7.430942	-7.431003	N/A	N/A	-7.626462	196	196	195	N/A	N/A	Al ₂ Sc + (Zr _{0.75} Sc _{0.25})B ₂ + Mn_{4/3}Sc_{2/3}AlB₂ + Mn ₂ B + AlMn
Ti	Sc	Fe	-7.276236	-7.276444	-7.276505	N/A	N/A	-7.550230	274	274	274	N/A	N/A	(Ti _{0.75} Sc _{0.25})B ₂ + Al ₆ Fe ₆ Sc + Fe_{4/3}Sc_{2/3}AlB₂ + Al ₆ Fe ₄ Sc + AlFe
Zr	Sc	Sc	-7.293796	-7.293737	-7.293908	-7.346520	-7.369598	-7.401148	107	107	107	55	32	(Zr _{0.5} Sc _{0.5})B ₂ + AlSc + (Zr _{0.75} Sc _{0.25})B ₂

Zr	Sc	Y	-7.216931	-7.216662	-7.216655	-7.246980	-7.300604	-7.412077	195	195	195	165	111	(Zr _{0.75} Sc _{0.25})B ₂ + (Zr _{0.5} Sc _{0.5})B ₂ + AlY ₂ + Al ₂ Y
Zr	Sc	Ti	-7.558015	-7.560805	-7.560659	-7.596167	-7.612539	-7.639677	82	79	79	44	27	(Zr _{0.83} Sc _{0.17}) ₄ AlB ₆ + Al ₃ Zr ₂ + (Ti _{0.83} Sc _{0.17}) ₄ AlB ₆ + AlSc + Al ₃ Zr ₄
Zr	Sc	Zr	-7.638981	-7.639149	-7.639150	N/A	-7.693072	-7.704542	66	65	65	N/A	11	Al ₃ Zr ₂ + AlSc + (Hf _{0.5} Zr _{0.5})B ₂ + (Hf _{0.75} Zr _{0.25})B ₂ + Al ₃ Zr ₄
Zr	Sc	Hf	-7.826940	-7.827106	-7.827093	-7.857260	-7.877084	-7.902135	75	75	75	45	25	Al ₃ Zr ₂ + (Hf _{0.5} Zr _{0.5})B ₂ + AlSc + Al ₃ Zr ₄
Zr	Sc	V	-7.605439	-7.606434	-7.605366	-7.653128	-7.673653	-7.762949	158	157	158	110	89	Al ₂ Sc + (Zr _{0.75} Sc _{0.25})B ₂ + VB + Al ₂ Zr
Zr	Sc	Nb	-7.773099	-7.772720	-7.772454	-7.835427	-7.856368	-7.870708	98	98	98	35	14	(Zr _{0.75} Sc _{0.25})B ₂ + NbB + Al ₂ Sc + Al ₂ Zr
Zr	Sc	Ta	-7.990625	-7.989966	-7.989706	-8.050820	-8.073477	-8.101149	111	111	111	50	28	(Zr _{0.75} Sc _{0.25})B ₂ + Al ₂ Sc + TaB + Al ₂ Zr
Zr	Sc	Cr	-7.522676	-7.525170	-7.524910	N/A	N/A	-7.757867	235	233	233	N/A	N/A	(Zr _{0.75} Sc _{0.25})B ₂ + Al ₃ Zr + CrB + Al ₃ Sc + Cr ₅ B ₃
Zr	Sc	Mo	-7.700566	-7.703820	-7.703763	N/A	N/A	-7.926431	226	223	223	N/A	N/A	Al ₈ Mo ₃ + (Zr _{0.75} Sc _{0.25})B ₂ + (Zr _{0.5} Sc _{0.5})B ₂ + AlMo ₃
Zr	Sc	W	-7.915759	-7.918229	-7.916160	N/A	N/A	-8.146740	231	229	231	N/A	N/A	Al ₅ W + (Zr _{0.75} Sc _{0.25})B ₂ + Al ₃ Sc + ScW ₂ B ₄ + W
Zr	Sc	Mn	-7.452156	-7.452930	-7.453014	N/A	N/A	-7.713993	262	261	261	N/A	N/A	Al ₂ Sc + Mn ₂ B + Mn _{4/3} Sc _{2/3} AlB ₂ + (Zr _{0.75} Sc _{0.25})B ₂ + AlMn
Zr	Sc	Fe	-7.296455	-7.296257	-7.296206	N/A	N/A	-7.638488	342	342	342	N/A	N/A	(Zr _{0.75} Sc _{0.25})B ₂ + (Zr _{0.5} Sc _{0.5})B ₂ + AlFe
Hf	Sc	Sc	-7.543102	-7.542923	-7.543346	-7.595918	-7.615446	-7.657091	114	114	114	61	42	(Hf _{0.5} Sc _{0.5})B ₂ + AlSc + (Hf _{0.75} Sc _{0.25})B ₂
Hf	Sc	Y	-7.463702	-7.463505	-7.463779	-7.485729	-7.537003	-7.668020	204	205	204	182	131	(Hf _{0.5} Sc _{0.5})B ₂ + AlY ₂ + Al ₂ Y + (Hf _{0.75} Sc _{0.25})B ₂
Hf	Sc	Ti	-7.810338	-7.810455	-7.810358	-7.852928	-7.863710	-7.884216	74	74	74	31	21	(Ti _{0.83} Sc _{0.17}) ₄ AlB ₆ + (Hf _{0.83} Sc _{0.17}) ₄ AlB ₆ + Al ₂ Sc + AlSc + Al ₃ Hf ₄
Hf	Sc	Zr	-7.884591	-7.884743	-7.884688	-7.919099	-7.937725	-7.962216	78	77	78	43	24	Al ₃ Zr ₂ + (Hf _{0.5} Zr _{0.5})B ₂ + AlSc + (Hf _{0.75} Zr _{0.25})B ₂ + Al ₃ Zr ₄
Hf	Sc	Hf	-8.072049	-8.072214	-8.072203	N/A	-8.122325	-8.134721	63	63	63	N/A	12	(Hf _{0.83} Sc _{0.17}) ₄ AlB ₆ + Al ₂ Sc + AlSc + Al ₃ Hf ₄
Hf	Sc	V	-7.857382	-7.857219	-7.857061	-7.913250	-7.926218	-8.010165	153	153	153	97	84	Al ₂ Sc + (Hf _{0.83} Sc _{0.17}) ₄ AlB ₆ + VB + Al ₃ Sc + (Hf _{0.75} Sc _{0.25})B ₂
Hf	Sc	Nb	-8.019146	-8.018443	-8.018160	-8.087181	-8.105123	-8.122452	103	104	104	35	17	NbB + Al ₃ Nb + (Nb _{0.75} Hf _{0.25})B ₂ + Al ₂ Sc + (Hf _{0.75} Sc _{0.25})B ₂
Hf	Sc	Ta	-8.235141	-8.234225	-8.233904	-8.301940	-8.321729	-8.348508	113	114	115	47	27	(Ta _{0.75} Hf _{0.25})B ₂ + Al ₃ Sc + (Hf _{0.75} Sc _{0.25})B ₂
Hf	Sc	Cr	-7.777378	-7.777396	-7.777177	N/A	N/A	-8.010381	233	233	233	N/A	N/A	Cr ₄ AlB ₄ + Al ₃ Sc + Cr ₅ B ₃ + AlCr ₂ + (Hf _{0.75} Sc _{0.25})B ₂
Hf	Sc	Mo	-7.953432	-7.952470	-7.952291	N/A	N/A	-8.182375	229	230	230	N/A	N/A	Al ₈ Mo ₃ + (Hf _{0.5} Sc _{0.5})B ₂ + AlMo ₃ + (Hf _{0.75} Sc _{0.25})B ₂
Hf	Sc	W	-8.160256	-8.164398	-8.164308	N/A	N/A	-8.401989	242	238	238	N/A	N/A	ScW ₂ B ₄ + Al ₃ Sc + Al ₅ W + (Hf _{0.75} Sc _{0.25})B ₂ + W
Hf	Sc	Mn	-7.703424	-7.704589	-7.704625	N/A	N/A	-7.969242	266	265	265	N/A	N/A	Mn _{4/3} Sc _{2/3} AlB ₂ + AlMn + Mn ₂ B + Al ₂ Sc + (Hf _{0.75} Sc _{0.25})B ₂
Hf	Sc	Fe	-7.546574	-7.546132	-7.545991	N/A	N/A	-7.894431	348	348	348	N/A	N/A	(Hf _{0.5} Sc _{0.5})B ₂ + AlFe + (Hf _{0.75} Sc _{0.25})B ₂
V	Sc	Sc	-7.383084	-7.383804	-7.383887	-7.378734	-7.383644	-7.421934	39	38	38	43	38	Al ₂ Sc + VB + ScB ₂ + (Sc _{0.75} V _{0.25})B ₂
V	Sc	Y	-7.277379	-7.279548	-7.278082	-7.220682	-7.275183	-7.394618	117	115	117	174	119	(Sc _{0.75} Y _{0.25})B ₂ + (V _{0.5} Y _{0.5})B ₂ + Al ₂ Y + VB + (Sc _{0.75} V _{0.25})B ₂
V	Sc	Ti	-7.663485	-7.661528	-7.661587	-7.668321	-7.647649	-7.708530	45	47	47	40	61	(Ti _{0.75} Sc _{0.25})B ₂ + Al ₃ Sc + VB
V	Sc	Zr	-7.703583	-7.701894	-7.701976	-7.663306	-7.674434	-7.774178	71	72	72	111	100	(Zr _{0.75} Sc _{0.25})B ₂ + Al ₃ Sc + VB
V	Sc	Hf	-7.896455	-7.894517	-7.894822	-7.861548	-7.867315	-7.965615	69	71	71	104	98	VB + Al ₃ Sc + (Hf _{0.75} Sc _{0.25})B ₂
V	Sc	V	-7.717388	-7.717424	-7.717377	N/A	-7.724249	-7.748542	31	31	31	N/A	24	(V _{0.5} Sc _{0.5})B ₂ + V ₃ B ₄ + Al ₃ Sc
V	Sc	Nb	-7.850816	-7.850975	-7.850881	-7.850888	-7.852656	-7.923858	73	73	73	73	71	Al ₃ Nb + VB + (Nb _{0.5} Sc _{0.5})B ₂
V	Sc	Ta	-8.069331	-8.069234	-8.069242	-8.070797	-8.071712	-8.126310	57	57	57	56	55	VB + Al ₃ Ta + (Ta _{0.5} Sc _{0.5})B ₂
V	Sc	Cr	-7.649416	-7.652416	-7.652518	N/A	N/A	-7.756114	107	104	104	N/A	N/A	Cr ₂ VAIB ₄ + (Cr _{0.5} V _{0.5})B + Cr ₂ V ₂ AlB ₆ + Al ₃ Sc + (V _{0.5} Sc _{0.5})B ₂
V	Sc	Mo	-7.814361	-7.818788	-7.819785	N/A	N/A	-7.928727	114	110	109	N/A	N/A	(V _{0.75} Sc _{0.25})B ₂ + (Mo _{0.5} V _{0.5})B + Al ₂₂ Mo ₅ + (V _{0.75} SMo _{0.25})B + (Sc _{0.75} Moc _{0.25})B ₂
V	Sc	W	-8.026959	-8.031946	-8.032175	N/A	N/A	-8.156720	130	125	125	N/A	N/A	(V _{0.75} Sc _{0.25})B ₂ + Al ₅ W + (V _{0.75} W _{0.25})B ₂ + (Sc _{0.75} W _{0.25})B ₂ + (W _{0.5} V _{0.5})B
V	Sc	Mn	-7.571283	-7.573173	-7.573254	N/A	N/A	-7.701225	130	129	129	N/A	N/A	Mn _{4/3} Sc _{2/3} VAIB ₄ + V ₃ B ₄ + Al ₁₁ Mn ₄ + (V _{0.5} Sc _{0.5})B ₂ + Mn _{4/3} Sc _{2/3} AlB ₂
V	Sc	Fe	-7.422539	-7.427348	-7.427501	N/A	N/A	-7.600330	178	177	177	N/A	N/A	V ₃ B ₄ + Fe _{4/3} Sc _{2/3} VAIB ₄ + (V _{0.75} Sc _{0.25})B ₂ + (V _{0.5} Sc _{0.5})B ₂ + Al ₈ Fe ₄ Sc
Nb	Sc	Sc	-7.563463	-7.563812	-7.564156	-7.594643	-7.615014	-7.619034	56	55	55	24	4	AlSc + (Nb _{0.5} Sc _{0.5}) ₄ AlB ₆
Nb	Sc	Y	-7.474641	-7.475394	-7.475656	-7.461015	-7.516241	-7.595663	121	117	117	131	76	(Nb _{0.5} Y _{0.5})B ₂ + AlY ₂ + Al ₂ Y + NbB + (Nb _{0.5} Sc _{0.5})B ₂
Nb	Sc	Ti	-7.822700	-7.821771	-7.821627	-7.842671	-7.853055	-7.860432	38	39	39	18	7	(Nb _{0.75} Ti _{0.25})B + (Nb _{0.5} Sc _{0.5}) ₄ AlB ₆ + Al ₃ Nb + Al ₂ Sc + TiB ₂
Nb	Sc	Zr	-7.885274	-7.884401	-7.884235	-7.884817	-7.911550	-7.921218	36	37	37	36	10	NbB + (Zr _{0.75} Sc _{0.25})B ₂ + (Nb _{0.5} Sc _{0.5}) ₄ AlB ₆ + Al ₂ Sc + Al ₃ Nb
Nb	Sc	Hf	-8.075380	-8.074510	-8.074362	-8.074570	-8.099563	-8.112655	37	38	38	38	13	NbB + Al ₃ Nb + (Nb _{0.5} Sc _{0.5}) ₄ AlB ₆ + Al ₂ Sc + (Hf _{0.75} Sc _{0.25})B ₂
Nb	Sc	V	-7.846453	-7.847871	-7.848022	-7.891148	-7.904735	-7.960336	114	112	112	69	56	(Nb _{0.75} V _{0.25})B + Al ₃ Nb + VB + (Nb _{0.5} Sc _{0.5})B ₂

Nb	Sc	Nb	-7.996256	-7.998871	-7.999138	N/A	-8.062111	-8.067538	71	69	68	N/A	5	Al ₃ Nb + NbB + (Nb _{0.5} Sc _{0.5})B ₂
Nb	Sc	Ta	-8.211857	-8.214393	-8.214597	-8.244518	-8.277255	-8.315379	104	101	101	71	38	(Nb _{0.5} Ta _{0.5})B + (Ta _{0.5} Sc _{0.5})B ₂ + Al ₃ Nb + (Nb _{0.5} Sc _{0.5})B ₂
Nb	Sc	Cr	-7.770873	-7.773152	-7.773212	N/A	N/A	-7.951375	181	178	178	N/A	N/A	Al ₃ Nb + CrB + NbB + (Nb _{0.5} Sc _{0.5})B ₂
Nb	Sc	Mo	-7.937878	-7.943926	-7.944256	N/A	N/A	-8.118352	180	174	174	N/A	N/A	Al ₈ Mo ₃ + (Nb _{0.75} Sc _{0.25})B ₂ + (Nb _{0.5} Mo _{0.5})B + (Nb _{0.5} Sc _{0.5})B ₂
Nb	Sc	W	-8.146930	-8.153395	-8.153868	N/A	N/A	-8.345245	198	192	191	N/A	N/A	(W _{0.75} Nb _{0.25})B + Al ₃ Nb + (Nb _{0.5} Sc _{0.5})B ₂
Nb	Sc	Mn	-7.701696	-7.702606	-7.702627	N/A	N/A	-7.886357	185	184	184	N/A	N/A	(Nb _{0.83} Sc _{0.17}) ₄ AlB ₆ + Mn _{4/3} Nb _{2/3} AlB ₂ + AlMn + (Nb _{0.5} Sc _{0.5})B ₂
Nb	Sc	Fe	-7.546249	-7.552628	-7.552945	N/A	N/A	-7.805212	259	253	252	N/A	N/A	(Nb _{0.75} Sc _{0.25})B ₂ + AlFe + (Nb _{0.5} Sc _{0.5})B ₂
Ta	Sc	Sc	-7.855109	-7.855603	-7.855846	-7.886359	-7.906737	-7.912230	57	57	56	26	5	AlSc + (Sc _{0.5} Ta _{0.5}) ₄ AlB ₆
Ta	Sc	Y	-7.765972	-7.766823	-7.766934	-7.751161	-7.801615	-7.895575	130	124	123	139	89	AlY ₂ + (Y _{0.5} Ta _{0.5})B ₂ + TaB + Al ₂ Y + (Ta _{0.5} Sc _{0.5})B ₂
Ta	Sc	Ti	-8.111079	-8.109805	-8.109740	-8.133930	-8.146476	-8.164540	53	55	55	31	18	(Ti _{0.75} Ta _{0.25})B ₂ + (Sc _{0.5} Ta _{0.5})B ₂ + (Ti _{0.75} Sc _{0.25})B ₂ + Al ₃ Sc + (Ta _{0.75} Ti _{0.25})B
Ta	Sc	Zr	-8.171422	-8.170157	-8.170160	-8.170757	-8.200923	-8.225113	54	55	55	54	24	(Zr _{0.75} Sc _{0.25})B ₂ + Al ₃ Sc + TaB
Ta	Sc	Hf	-8.360569	-8.359297	-8.359347	-8.359957	-8.388371	-8.416549	56	57	57	57	28	Al ₃ Sc + TaB + (Hf _{0.75} Sc _{0.25})B ₂
Ta	Sc	V	-8.134093	-8.135162	-8.135325	-8.182224	-8.195469	-8.242330	108	107	107	60	47	(V _{0.75} Ta _{0.25})B + Al ₃ Ta + (Ta _{0.5} Sc _{0.5})B ₂
Ta	Sc	Nb	-8.280054	-8.282179	-8.282301	-8.315613	-8.349115	-8.389210	109	107	107	74	40	(Nb _{0.5} Ta _{0.5})B + (Ta _{0.5} Sc _{0.5})B ₂ + Al ₃ Nb
Ta	Sc	Ta	-8.493815	-8.495500	-8.495637	N/A	-8.561822	-8.577245	83	82	82	N/A	15	(Ta _{0.5} Sc _{0.5})B ₂ + Al ₃ Ta + TaB
Ta	Sc	Cr	-8.059495	-8.061365	-8.061429	N/A	N/A	-8.234857	175	173	173	N/A	N/A	Cr ₄ AlB ₄ + CrTa ₂ B ₂ + Al ₃ Ta + (Ta _{0.5} Sc _{0.5})B ₂ + TaB
Ta	Sc	Mo	-8.221147	-8.226323	-8.226704	N/A	N/A	-8.418605	197	192	192	N/A	N/A	(Mo _{0.5} Ta _{0.5})B + Al ₈ Mo ₃ + Al ₂₂ Mo ₅ + (Ta _{0.5} Sc _{0.5})B ₂
Ta	Sc	W	-8.426707	-8.432268	-8.432542	N/A	N/A	-8.633044	206	201	201	N/A	N/A	Al ₅ W + (W _{0.75} Ta _{0.25})B + Al ₃ Sc + (W _{0.5} Ta _{0.5})B + (Ta _{0.5} Sc _{0.5})B ₂
Ta	Sc	Mn	-7.990170	-7.991267	-7.991367	N/A	N/A	-8.184274	194	193	193	N/A	N/A	Al ₁₁ Mn ₄ + (Ta _{0.5} Sc _{0.5})B ₂ + AlMn + Mn ₂ AlB ₂ + TaB
Ta	Sc	Fe	-7.833441	-7.839643	-7.839863	N/A	N/A	-8.090146	257	251	250	N/A	N/A	(Ta _{0.5} Sc _{0.5})B ₂ + (Ta _{0.75} Sc _{0.25})B ₂ + AlFe
Cr	Sc	Sc	-7.396780	-7.396613	-7.396740	-7.338179	-7.344597	-7.413217	16	17	16	75	69	Cr _{4/3} Sc _{2/3} AlB ₂ + ScB ₂
Cr	Sc	Y	-7.287182	-7.286742	-7.286805	-7.175148	-7.248858	-7.397714	111	111	111	223	149	AlY ₂ + CrYB ₄ + Al ₂ Y + CrB + ScB ₂
Cr	Sc	Ti	-7.675090	-7.675099	-7.675092	-7.626932	-7.598931	-7.697327	22	22	22	70	98	(Ti _{0.75} Sc _{0.25})B ₂ + Al ₃ Sc + CrB
Cr	Sc	Zr	-7.710022	-7.709883	-7.709793	-7.607696	-7.623979	-7.762975	53	53	53	155	139	(Zr _{0.75} Sc _{0.25})B ₂ + CrB + Al ₃ Sc
Cr	Sc	Hf	-7.903194	-7.903192	-7.903155	-7.807112	-7.810325	-7.954411	51	51	51	147	144	CrB + Al ₃ Sc + (Hf _{0.75} Sc _{0.25})B ₂
Cr	Sc	V	-7.736400	-7.738330	-7.738279	-7.721241	-7.680042	-7.752030	16	14	14	31	72	Cr ₂ VAIB ₄ + (Cr _{0.75} V _{0.25})B + Al ₃ Sc + (Sc _{0.5} V _{0.5})B ₂
Cr	Sc	Nb	-7.863217	-7.864978	-7.864833	-7.803544	-7.793721	-7.912655	49	48	48	109	119	Al ₃ Nb + CrB + (Nb _{0.5} Sc _{0.5})B ₂
Cr	Sc	Ta	-8.081795	-8.083425	-8.083210	-8.022701	-8.011078	-8.120583	39	37	37	98	110	Cr ₄ AlB ₄ + CrTa ₂ B ₂ + Al ₃ Ta + (Ta _{0.5} Sc _{0.5})B ₂ + Al ₃ Sc
Cr	Sc	Cr	-7.674944	-7.680315	-7.679518	N/A	N/A	-7.716110	41	36	37	N/A	N/A	Cr ₂ AlB ₂ + CrSc ₂ B ₆
Cr	Sc	Mo	-7.836714	-7.841716	-7.841684	N/A	N/A	-7.900421	64	59	59	N/A	N/A	Cr ₄ AlB ₄ + (Sc _{0.75} Mo _{0.25})B ₂ + (Sc _{0.5} Mo _{0.5})B ₂ + MoAlB
Cr	Sc	W	-8.048613	-8.053616	-8.053574	N/A	N/A	-8.121657	73	68	68	N/A	N/A	(Sc _{0.75} W _{0.25})B ₂ + (Cr _{0.5} W _{0.5})AlB + Cr ₂ AlB ₂ + (Cr _{0.5} W _{0.5})B + (W _{0.75} Cr _{0.25})B ₂
Cr	Sc	Mn	-7.591401	-7.595004	-7.594879	N/A	N/A	-7.688431	97	93	94	N/A	N/A	(Cr _{0.67} Mn _{0.33}) ₂ AlB ₂ + CrSc ₂ B ₆ + (Mn _{0.67} Cr _{0.33}) ₂ AlB ₂
Cr	Sc	Fe	-7.446398	-7.451169	-7.451529	N/A	N/A	-7.569757	123	119	118	N/A	N/A	(Cr _{0.67} Fe _{0.33}) ₂ AlB ₂ + (Fe _{0.67} Cr _{0.33}) ₂ AlB ₂ + CrSc ₂ B ₆
Mo	Sc	Sc	-7.636183	-7.635686	-7.635712	-7.610881	-7.636049	-7.645625	9	10	10	35	10	Al ₈ Mo ₃ + Al ₂ Sc + (Sc _{0.75} Mo _{0.25})B ₂ + AlMo ₃
Mo	Sc	Y	-7.536687	-7.536270	-7.536355	-7.467035	-7.528836	-7.611921	75	76	76	145	83	MoYB ₄ + AlY ₂ + Al ₂ Y + Mo _{4/3} Y _{2/3} AlB ₂ + (Sc _{0.75} Mo _{0.25})B ₂
Mo	Sc	Ti	-7.888716	-7.887848	-7.887761	-7.859616	-7.868382	-7.912129	23	24	24	53	44	(Mo _{0.75} Ti _{0.25})B + (Ti _{0.75} Sc _{0.25})B ₂ + Al ₈ Mo ₃ + (Sc _{0.75} Mo _{0.25})B ₂ + AlMo ₃
Mo	Sc	Zr	-7.938071	-7.937548	-7.937566	-7.875694	-7.909586	-7.972355	34	35	35	97	63	Al ₈ Mo ₃ + (Zr _{0.75} Sc _{0.25})B ₂ + (Sc _{0.75} Mo _{0.25})B ₂ + AlMo ₃ + MoB
Mo	Sc	Hf	-8.130064	-8.129450	-8.129404	-8.069265	-8.098387	-8.163792	34	34	34	95	65	Al ₈ Mo ₃ + (Sc _{0.75} Mo _{0.25})B ₂ + AlMo ₃ + MoB + (Hf _{0.75} Sc _{0.25})B ₂
Mo	Sc	V	-7.922852	-7.928832	-7.928875	-7.922737	-7.922566	-7.975225	52	46	46	52	53	(V _{0.75} Sc _{0.25})B ₂ + MoAlB + (Mo _{0.5} V _{0.5})B + Al ₂₂ Mo ₅ + (Sc _{0.75} Mo _{0.25})B ₂
Mo	Sc	Nb	-8.061278	-8.067608	-8.067717	-8.035246	-8.057655	-8.124916	64	57	57	90	67	Al ₈ Mo ₃ + (Nb _{0.75} Sc _{0.25})B ₂ + (Mo _{0.75} Nb _{0.25})B + MoAlB + (Nb _{0.5} Sc _{0.5})B ₂
Mo	Sc	Ta	-8.277737	-8.283753	-8.283986	-8.249426	-8.269817	-8.348808	71	65	65	99	79	(Mo _{0.75} Ta _{0.25})B + MoAlB + (Mo _{0.5} Ta _{0.5})B + Al ₈ Mo ₃ + (Ta _{0.5} Sc _{0.5})B ₂
Mo	Sc	Cr	-7.853774	-7.858772	-7.858290	N/A	N/A	-7.951223	97	92	93	N/A	N/A	Cr ₄ AlB ₄ + (Cr _{0.75} Mo _{0.25})B + (Sc _{0.75} Mo _{0.25})B ₂ + (Mo _{0.5} Sc _{0.5})B ₂ + MoAlB
Mo	Sc	Mo	-8.018755	-8.024461	-8.024057	N/A	N/A	-8.092895	74	68	69	N/A	N/A	(Mo _{0.5} Sc _{0.5})B ₂ + Mo ₄ AlB ₄ + (Sc _{0.75} Mo _{0.25})B ₂ + MoAlB
Mo	Sc	W	-8.226305	-8.233224	-8.233118	N/A	N/A	-8.344412	118	111	111	N/A	N/A	(Mo _{0.5} Sc _{0.5})B ₂ + (Mo _{0.5} W _{0.5})AlB + (Mo _{0.5} W _{0.5})B + (Sc _{0.75} Mo _{0.25})B ₂

Mo	Sc	Mn	-7.772469	-7.775606	-7.775469	N/A	N/A	-7.883553	111	108	108	N/A	N/A	(Mo _{0.5} Sc _{0.5})B ₂ + (Mn _{0.67} Mo _{0.33}) ₂ AlB ₂ + (Mo _{0.67} Mn _{0.33}) ₂ AlB ₂ + (Sc _{0.75} Mo _{0.25})B ₂
Mo	Sc	Fe	-7.624461	-7.629199	-7.628866	N/A	N/A	-7.773869	149	145	145	N/A	N/A	(Mo _{0.5} Sc _{0.5})B ₂ + Mo ₄ AlB ₄ + Fe ₂ AlB ₂ + (Sc _{0.75} Mo _{0.25})B ₂ + MoAlB
W	Sc	Sc	-7.945337	-7.944262	-7.944192	-7.910898	-7.940809	-7.957116	12	13	13	46	16	ScW ₂ B ₄ + (Sc _{0.75} W _{0.25})B ₂ + Al ₃ Sc + W
W	Sc	Y	-7.845212	-7.844389	-7.844441	-7.762235	-7.826007	-7.919765	75	75	75	158	94	W _{4/3} Y _{2/3} AlB ₂ + ScW ₂ B ₄ + (Sc _{0.75} W _{0.25})B ₂ + WY ₃ B ₇ + Al ₂ Y
W	Sc	Ti	-8.190555	-8.189204	-8.189036	-8.153938	-8.168291	-8.214452	24	25	25	61	46	(W _{0.75} Ti _{0.25})B + (Ti _{0.75} Sc _{0.25})B ₂ + Al ₃ Sc + Al ₅ W + (Sc _{0.75} W _{0.25})B ₂
W	Sc	Zr	-8.238201	-8.237590	-8.237594	-8.167227	-8.206315	-8.270158	32	33	33	103	64	Al ₅ W + (Zr _{0.75} Sc _{0.25})B ₂ + ScW ₂ B ₄ + W
W	Sc	Hf	-8.428798	-8.428112	-8.428050	-8.359045	-8.393589	-8.461595	33	33	34	103	68	ScW ₂ B ₄ + Al ₅ W + (Hf _{0.75} Sc _{0.25})B ₂ + W
W	Sc	V	-8.218472	-8.223845	-8.223846	-8.213196	-8.216547	-8.279068	61	55	55	66	63	(Sc _{0.75} V _{0.25})B ₂ + Al ₅ W + (Sc _{0.75} W _{0.25})B ₂ + VWB ₂ + (W _{0.75} V _{0.25})B
W	Sc	Nb	-8.351657	-8.358154	-8.358221	-8.321054	-8.347397	-8.417738	66	60	60	97	70	Al ₅ W + (W _{0.75} Nb _{0.25})B + Al ₃ Nb + ScW ₂ B ₄ + (Nb _{0.5} Sc _{0.5})B ₂
W	Sc	Ta	-8.565005	-8.571421	-8.571584	-8.531263	-8.555512	-8.639139	74	68	68	108	84	Al ₅ W + (W _{0.75} Ta _{0.25})B + Al ₃ Sc + (Ta _{0.5} Sc _{0.5})B ₂
W	Sc	Cr	-8.144799	-8.151202	-8.150828	N/A	N/A	-8.248109	103	97	97	N/A	N/A	(Sc _{0.75} W _{0.25})B ₂ + (Cr _{0.5} W _{0.5})AlB + (W _{0.75} Cr _{0.25})B + (W _{0.5} Cr _{0.5})B + (W _{0.75} Cr _{0.25})B ₂
W	Sc	Mo	-8.303310	-8.310232	-8.309782	N/A	N/A	-8.422065	119	112	112	N/A	N/A	(Mo _{0.5} W _{0.5})B ₂ + (Mo _{0.5} W _{0.5})AlB + (W _{0.75} Mo _{0.25})B + (Sc _{0.75} W _{0.25})B ₂ + (W _{0.5} Mo _{0.5})B
W	Sc	W	-8.506065	-8.514246	-8.514045	N/A	N/A	-8.608990	103	95	95	N/A	N/A	ScW ₂ B ₄ + (Sc _{0.75} W _{0.25})B ₂ + WB ₂ + WAlB
W	Sc	Mn	-8.068036	-8.070293	-8.070069	N/A	N/A	-8.179287	111	109	109	N/A	N/A	(Sc _{0.75} W _{0.25})B ₂ + WB ₂ + (W _{0.75} Mn _{0.25})B + WAlB + Mn ₂ AlB ₂
W	Sc	Fe	-7.916408	-7.923975	-7.923546	N/A	N/A	-8.070109	154	146	147	N/A	N/A	WB ₂ + Fe ₂ AlB ₂ + (Sc _{0.75} W _{0.25})B ₂ + FeW ₂ B ₂ + WAlB
Mn	Sc	Sc	-7.338919	-7.337959	-7.337902	-7.235451	-7.248183	-7.364552	26	27	27	129	116	Mn _{4/3} Sc _{2/3} AlB ₂ + ScB ₂
Mn	Sc	Y	-7.225608	-7.224257	-7.224237	-7.093372	-7.158548	-7.315524	90	91	91	222	157	MnYB ₄ + Mn _{4/3} Y _{2/3} AlB ₂ + MnY ₃ B ₇ + Al ₂ Y + ScB ₂
Mn	Sc	Ti	-7.617196	-7.617822	-7.618077	-7.524918	-7.489816	-7.641132	24	23	23	116	151	Mn _{4/3} Sc _{2/3} AlB ₂ + TiB ₂
Mn	Sc	Zr	-7.647592	-7.647553	-7.647686	-7.507235	-7.530411	-7.706144	59	59	58	199	176	Mn _{4/3} Zr _{2/3} AlB ₂ + Mn _{4/3} Sc _{2/3} AlB ₂ + (Zr _{0.75} Sc _{0.25})B ₂
Mn	Sc	Hf	-7.841405	-7.841596	-7.841835	-7.704752	-7.713066	-7.891912	51	50	50	187	179	Mn _{4/3} Hf _{2/3} AlB ₂ + Mn _{4/3} Sc _{2/3} AlB ₂ + (Hf _{0.75} Sc _{0.25})B ₂
Mn	Sc	V	-7.682549	-7.684165	-7.684374	-7.626694	-7.574639	-7.680905	-2	-3	-3	54	106	Mn _{4/3} Sc _{2/3} V ₂ AlB ₆ + Mn _{4/3} Sc _{2/3} AlB ₂
Mn	Sc	Nb	-7.802327	-7.804322	-7.804515	-7.703656	-7.688196	-7.825235	23	21	21	122	137	Mn _{4/3} Nb _{2/3} AlB ₂ + AlMn + Mn ₂ AlB ₂ + (Nb _{0.5} Sc _{0.5})B ₂
Mn	Sc	Ta	-8.019957	-8.022052	-8.022167	-7.921557	-7.903862	-8.047357	27	25	25	126	143	Al ₁₁ Mn ₄ + (Ta _{0.5} Sc _{0.5})B ₂ + AlMn + Mn ₂ AlB ₂ + TaB
Mn	Sc	Cr	-7.625443	-7.631383	-7.631533	N/A	N/A	-7.667442	42	36	36	N/A	N/A	CrSc ₂ B ₆ + (Mn _{0.67} Cr _{0.33}) ₂ AlB ₂
Mn	Sc	Mo	-7.779089	-7.788355	-7.787993	N/A	N/A	-7.812994	34	25	25	N/A	N/A	(Mo _{0.5} Sc _{0.5})B ₂ + (Mn _{0.67} Mo _{0.33}) ₂ AlB ₂ + (Sc _{0.75} Mo _{0.25})B ₂
Mn	Sc	W	-7.989009	-7.999351	-7.998956	N/A	N/A	-8.035353	46	36	36	N/A	N/A	(Sc _{0.75} W _{0.25})B ₂ + WB ₂ + (W _{0.75} Mn _{0.25})B + WAlB + Mn ₂ AlB ₂
Mn	Sc	Mn	-7.532393	-7.535312	-7.535433	N/A	N/A	-7.559749	27	24	24	N/A	N/A	MnB ₄ + Mn ₄ AlB ₄ + (Sc _{0.75} Mn _{0.25})B ₂ + Mn ₂ AlB ₂
Mn	Sc	Fe	-7.378495	-7.387575	-7.388149	N/A	N/A	-7.476446	98	89	88	N/A	N/A	(Mn _{0.67} Fe _{0.33}) ₂ AlB ₂ + (Fe _{0.67} Mn _{0.33}) ₂ AlB ₂ + (Sc _{0.75} Mn _{0.25})B ₂ + MnB ₄ + FeB
Fe	Sc	Sc	-7.200915	-7.201942	-7.201714	-7.057893	-7.093300	-7.221297	20	19	20	163	128	Fe _{4/3} Sc _{2/3} AlB ₂ + ScB ₂
Fe	Sc	Y	-7.088211	-7.088290	-7.088297	-6.937759	-7.012469	-7.175713	88	87	87	238	163	FeYB ₄ + Fe _{4/3} Y _{2/3} AlB ₂ + Fe ₂ YB ₂ + Al ₂ Y + ScB ₂
Fe	Sc	Ti	-7.471712	-7.473218	-7.472722	-7.345262	-7.320553	-7.501038	29	28	28	156	180	(Ti _{0.75} Sc _{0.25})B ₂ + Fe _{4/3} Sc _{2/3} AlB ₂ + Fe ₂ AlB ₂ + AlFe
Fe	Sc	Zr	-7.497885	-7.497726	-7.497617	-7.326223	-7.363308	-7.566686	69	69	69	240	203	(Zr _{0.75} Sc _{0.25})B ₂ + AlFe + Fe _{4/3} Sc _{2/3} AlB ₂ + Fe ₂ AlB ₂
Fe	Sc	Hf	-7.693128	-7.692931	-7.692784	-7.522848	-7.542936	-7.758122	65	65	65	235	215	Fe _{4/3} Sc _{2/3} AlB ₂ + AlFe + Fe ₂ AlB ₂ + (Hf _{0.75} Sc _{0.25})B ₂
Fe	Sc	V	-7.540354	-7.546510	-7.546631	-7.452696	-7.403532	-7.537010	-3	-10	-10	84	133	Fe _{4/3} Sc _{2/3} V ₂ AlB ₆ + Fe _{4/3} Sc _{2/3} AlB ₂
Fe	Sc	Nb	-7.654976	-7.658159	-7.657991	-7.521767	-7.517065	-7.699700	45	42	42	178	183	(Nb _{0.75} Sc _{0.25})B ₂ + Fe ₂ AlB ₂ + AlFe + (Nb _{0.5} Sc _{0.5})B ₂
Fe	Sc	Ta	-7.873325	-7.876361	-7.876060	-7.739031	-7.727601	-7.915998	43	40	40	177	188	(Ta _{0.5} Sc _{0.5})B ₂ + Fe ₂ AlB ₂ + (Ta _{0.75} Sc _{0.25})B ₂ + AlFe
Fe	Sc	Cr	-7.471766	-7.473203	-7.473285	N/A	N/A	-7.513211	41	40	40	N/A	N/A	(Fe _{0.67} Cr _{0.33}) ₂ AlB ₂ + CrSc ₂ B ₆
Fe	Sc	Mo	-7.628078	-7.631014	-7.631006	N/A	N/A	-7.667527	39	37	37	N/A	N/A	(Mo _{0.5} Sc _{0.5})B ₂ + Mo ₄ AlB ₄ + Fe ₂ AlB ₂ + (Sc _{0.75} Mo _{0.25})B ₂ + MoAlB
Fe	Sc	W	-7.840026	-7.843026	-7.843160	N/A	N/A	-7.890415	50	47	47	N/A	N/A	WB ₂ + Fe ₂ AlB ₂ + (Sc _{0.75} W _{0.25})B ₂ + FeW ₂ B ₂ + WAlB
Fe	Sc	Mn	-7.379220	-7.380683	-7.380661	N/A	N/A	-7.440375	61	60	60	N/A	N/A	(Mn _{0.67} Fe _{0.33}) ₂ AlB ₂ + (Fe _{0.67} Mn _{0.33}) ₂ AlB ₂ + (Sc _{0.75} Mn _{0.25})B ₂ + MnB ₄ + FeB
Fe	Sc	Fe	-7.216704	-7.221820	-7.221354	N/A	N/A	-7.299483	83	78	78	N/A	N/A	Fe ₂ B ₇ + Fe ₂ AlB ₂ + FeB + ScB ₂

Table S3. Calculated energy (E) and stability at 2000 K (ΔG_{cp}^{s-MAB} , $\Delta G_{cp}^{partial\ disorder}$, $\Delta G_{cp}^{disorder}$) for M2 = Y in *s*-MAB, *s*-MAB with disorder, and MAB with disorder for 314 MAB phases along with corresponding energy for their competing phases and identified set of most competing phases. Phases modelled with solid solution disorder have a contribution from configurational entropy evaluated at 2000 K. Competing phases in bold highlight when a MAB phase is part of the set of most competing phases.

M1	M2	M3	Energy (eV/atom)					ΔG_{cp} (meV/atom)					Set of most competing phases	
			s-MAB (no. 191)	s-MAB (no. 194)	s-MAB (no. 166)	s-MAB disorder	MAB disorder	Competing phases	s-MAB (no. 191)	s-MAB (no. 194)	s-MAB (no. 166)	s-MAB partial disorder		MAB disorder
Sc	Y	Sc	-6.890317	-6.890485	-6.890347	N/A	-6.898277	-6.930884	41	40	41	N/A	33	AlSc ₂ + AlY ₂ + Al ₂ Y + ScB ₂
Sc	Y	Y	-6.814570	-6.814941	-6.814902	-6.821454	-6.823614	-6.881327	67	66	66	60	58	(Sc _{0.75} Y _{0.25})B ₂ + (Y _{0.75} Sc _{0.25})B ₂ + AlY ₂ + Al ₂ Y
Sc	Y	Ti	-7.156917	-7.156451	-7.156329	-7.180359	-7.135564	-7.225196	68	69	69	45	90	(Sc _{0.5} Ti _{0.5})B ₂ + AlY ₂ + AlSc ₂ + Al ₂ Y
Sc	Y	Zr	-7.237489	-7.237228	-7.237082	-7.250191	-7.218838	-7.298124	61	61	61	48	79	(Sc _{0.5} Zr _{0.5})B ₂ + AlSc ₂ + AlY ₂ + Al ₂ Y
Sc	Y	Hf	-7.427250	-7.426865	-7.426723	-7.436599	-7.399073	-7.491643	64	65	65	55	93	(Sc _{0.5} Hf _{0.5})B ₂ + AlSc ₂ + AlY ₂ + Al ₂ Y
Sc	Y	V	-7.208518	-7.209598	-7.209610	-7.258900	-7.206274	-7.310678	102	101	101	52	104	AlY ₂ + Al ₂ Y + VB + ScB ₂ + (Sc _{0.75} V _{0.25})B ₂
Sc	Y	Nb	-7.385360	-7.386754	-7.386696	-7.436788	-7.390768	-7.461803	76	75	75	25	71	(Sc _{0.75} Nb _{0.25})B ₂ + AlY ₂ + (Nb_{0.5}Sc_{0.5})₄AlB₆ + Al ₂ Y + (Sc _{0.5} Nb _{0.5})B ₂
Sc	Y	Ta	-7.607268	-7.608516	-7.608476	-7.655447	-7.607059	-7.688271	81	80	80	33	81	AlY ₂ + (Sc _{0.75} Ta _{0.25})B ₂ + TaB + AlSc ₂ + Al ₂ Y
Sc	Y	Cr	-7.135496	-7.134881	-7.134681	N/A	N/A	-7.300407	165	166	166	N/A	N/A	AlY ₂ + CrYB ₄ + Al ₂ Y + CrB + ScB ₂
Sc	Y	Mo	-7.342366	-7.343087	-7.343283	N/A	N/A	-7.478500	136	135	135	N/A	N/A	AlMo ₃ + AlY ₂ + Al ₂ Y + Mo_{4/3}Y_{2/3}AlB₂ + (Sc _{0.75} Mo _{0.25})B ₂
Sc	Y	W	-7.565570	-7.566185	-7.566391	N/A	N/A	-7.718814	153	153	152	N/A	N/A	ScW ₂ B ₄ + (Sc _{0.75} W _{0.25})B ₂ + WY ₃ B ₇ + Al ₂ Y + W
Sc	Y	Mn	-7.060998	-7.061719	-7.061720	N/A	N/A	-7.241750	181	180	180	N/A	N/A	Mn_{4/3}Y_{2/3}AlB₂ + AlY ₂ + Al ₂ Y + Mn ₂ B + ScB ₂
Sc	Y	Fe	-6.913953	-6.913600	-6.913598	N/A	N/A	-7.139418	225	226	226	N/A	N/A	Al ₆ Fe ₆ Sc + Fe_{4/3}Y_{2/3}AlB₂ + Fe ₂ YB ₂ + Al ₂ Y + ScB ₂
Y	Y	Sc	N/A	N/A	N/A	N/A	-6.812964	-6.853739	N/A	N/A	N/A	N/A	41	(Sc _{0.75} Y _{0.25})B ₂ + (Y _{0.75} Sc _{0.25})B ₂ + AlY ₂ + Al ₂ Y
Y	Y	Ti	N/A	N/A	N/A	N/A	-7.032583	-7.124328	N/A	N/A	N/A	N/A	92	AlY ₂ + YB ₂ + Al ₂ Y + TiB ₂
Y	Y	Zr	N/A	N/A	N/A	N/A	-7.139287	-7.198950	N/A	N/A	N/A	N/A	60	(Zr _{0.5} Y _{0.5})B ₂ + AlY ₂ + Al ₂ Y
Y	Y	Hf	N/A	N/A	N/A	N/A	-7.313876	-7.380122	N/A	N/A	N/A	N/A	66	(Y _{0.75} Hf _{0.25})B ₂ + (Hf _{0.75} Y _{0.25})B ₂ + AlY ₂ + Al ₂ Y
Y	Y	V	N/A	N/A	N/A	N/A	-7.094916	-7.191884	N/A	N/A	N/A	N/A	97	VYB ₄ + AlY ₂ + Al ₂ Y
Y	Y	Nb	N/A	N/A	N/A	N/A	-7.294067	-7.326802	N/A	N/A	N/A	N/A	33	(Nb _{0.5} Y _{0.5})B ₂ + AlY ₂ + Al ₂ Y
Y	Y	Ta	N/A	N/A	N/A	N/A	-7.506066	-7.541995	N/A	N/A	N/A	N/A	36	(Y _{0.75} Ta _{0.25})B ₂ + AlY ₂ + Al ₂ Y + TaB
Ti	Y	Sc	-7.237161	-7.236705	-7.236837	-7.270155	-7.213347	-7.318801	82	82	82	49	105	(Sc _{0.5} Ti _{0.5})B ₂ + (Ti _{0.75} Sc _{0.25})B ₂ + AlY ₂ + AlSc ₂ + Al ₂ Y
Ti	Y	Y	-7.149022	-7.148979	-7.149086	-7.135295	-7.123694	-7.245339	96	96	96	110	122	AlY ₂ + YB ₂ + Al ₂ Y + TiB ₂
Ti	Y	Ti	-7.513123	-7.513932	-7.513964	N/A	-7.465711	-7.551074	38	37	37	N/A	85	Ti ₃ B ₄ + AlY ₂ + Al ₂ Y + TiB ₂
Ti	Y	Zr	-7.577300	-7.577910	-7.577896	-7.581793	-7.526607	-7.619131	42	41	41	37	93	(Zr _{0.75} Ti _{0.25})B ₂ + AlY ₂ + Al ₃ Zr ₄ + Al ₂ Y + TiB ₂
Ti	Y	Hf	-7.767375	-7.768077	-7.768097	-7.774460	-7.712337	-7.807853	40	40	40	33	96	(Ti _{0.75} Hf _{0.25})B ₂ + (Hf _{0.5} Ti _{0.5})B ₂ + AlY ₂ + Al ₂ Y + Al ₃ Hf ₄
Ti	Y	V	-7.569798	-7.570349	-7.570478	-7.625592	-7.536632	-7.676166	106	106	106	51	140	(Ti _{0.75} V _{0.25})B ₂ + AlY ₂ + Al ₂ Y + VB + TiB ₂
Ti	Y	Nb	-7.724824	-7.724724	-7.724786	-7.768119	-7.699102	-7.794556	70	70	70	26	95	(Nb _{0.75} Ti _{0.25}) ₅ B ₆ + (Ti _{0.75} Nb _{0.25})B ₂ + AlY ₂ + Al ₂ Y
Ti	Y	Ta	-7.943288	-7.942986	-7.943122	-7.986848	-7.916114	-8.022621	79	80	79	36	107	(Nb _{0.75} Ti _{0.25}) ₅ B ₆ + AlY ₂ + (Ti _{0.75} Ta _{0.25})B ₂ + Al ₂ Y
Ti	Y	Cr	-7.496178	-7.496854	-7.496820	N/A	N/A	-7.669179	173	172	172	N/A	N/A	AlY ₂ + CrYB ₄ + CrB + Al ₂ Y + TiB ₂
Ti	Y	Mo	-7.678943	-7.676940	-7.676759	N/A	N/A	-7.825859	147	149	149	N/A	N/A	(Mo _{0.75} Ti _{0.25})B + AlY ₂ + Mo_{4/3}Y_{2/3}AlB₂ + Al ₂ Y + TiB ₂
Ti	Y	W	-7.894601	-7.892532	-7.892385	N/A	N/A	-8.055477	161	163	163	N/A	N/A	W_{4/3}Y_{2/3}AlB₂ + (W _{0.75} Ti _{0.25})B + WY ₃ B ₇ + Al ₂ Y + TiB ₂
Ti	Y	Mn	-7.422390	-7.422954	-7.422881	N/A	N/A	-7.610522	188	188	188	N/A	N/A	Mn ₂ B + AlY ₂ + Mn_{4/3}Y_{2/3}AlB₂ + Al ₂ Y + TiB ₂
Ti	Y	Fe	-7.268682	-7.268734	-7.268887	N/A	N/A	-7.507952	239	239	239	N/A	N/A	Al ₈ Fe ₄ Y + Fe_{4/3}Y_{2/3}AlB₂ + Fe ₂ YB ₂ + Al ₂ Y + TiB ₂

Zr	Y	Sc	-7.299944	-7.299736	-7.299972	-7.359502	-7.326521	-7.408758	109	109	109	49	82	(Zr _{0.75} Sc _{0.25})B ₂ + (Sc _{0.5} Zr _{0.5})B ₂ + AlSc ₂ + AlY ₂ + Al ₂ Y
Zr	Y	Y	-7.230535	-7.230509	-7.230639	-7.263644	-7.259429	-7.340583	110	110	110	77	81	(Zr _{0.5} Y _{0.5})B ₂ + (Zr _{0.75} Y _{0.25})B ₂ + AlY ₂ + Al ₂ Y
Zr	Y	Ti	-7.560154	-7.561027	-7.561073	-7.601984	-7.555044	-7.638646	78	78	78	37	84	(Zr _{0.75} Ti _{0.25})B ₂ + AlY ₂ + Al ₃ Zr ₄ + Al ₂ Y + TiB ₂
Zr	Y	Zr	-7.648723	-7.649647	-7.649660	N/A	-7.649045	-7.692137	43	42	42	N/A	43	AlY ₂ + Al ₃ Zr ₄ + Al ₂ Y + ZrB ₂
Zr	Y	Hf	-7.834847	-7.835856	-7.835751	-7.867050	-7.828611	-7.910269	75	74	75	43	82	AlY ₂ + (Zr _{0.5} Zr _{0.5})B ₂ + Al ₂ Y + Al ₃ Zr ₄
Zr	Y	V	-7.603266	-7.603790	-7.603662	-7.653896	-7.607741	-7.754326	151	151	151	100	147	(Zr _{0.75} Y _{0.25})B ₂ + Al ₂ Y + VB + ZrB ₂
Zr	Y	Nb	-7.779643	-7.779645	-7.779496	-7.838967	-7.797939	-7.862151	83	83	83	23	64	(Zr _{0.75} Nb _{0.25})B ₂ + AlY ₂ + Al ₂ Y + NbB + ZrB ₂
Zr	Y	Ta	-7.996355	-7.996328	-7.996192	-8.052960	-8.012167	-8.092527	96	96	96	40	80	(Zr _{0.75} Y _{0.25})B ₂ + Al ₂ Y + TaB + ZrB ₂
Zr	Y	Cr	-7.524608	-7.525684	-7.525587	N/A	N/A	-7.745923	221	220	220	N/A	N/A	(Zr _{0.75} Y _{0.25})B ₂ + CrB + Al ₂ Y + ZrB ₂
Zr	Y	Mo	-7.711438	-7.710357	-7.710207	N/A	N/A	-7.898688	187	188	188	N/A	N/A	AlY ₂ + Mo _{4/3} Y _{2/3} AlB ₂ + AlMo ₃ + Al ₂ Y + ZrB ₂
Zr	Y	W	-7.925624	-7.924801	-7.924657	N/A	N/A	-8.127739	202	203	203	N/A	N/A	W _{4/3} Y _{2/3} AlB ₂ + (Zr _{0.75} Y _{0.25})B ₂ + Al ₂ Y + ZrB ₂ + W
Zr	Y	Mn	-7.454757	-7.455358	-7.455497	N/A	N/A	-7.685917	231	231	230	N/A	N/A	(Zr _{0.75} Y _{0.25})B ₂ + Mn ₂ B + Mn _{4/3} Y _{2/3} AlB ₂ + Al ₂ Y + ZrB ₂
Zr	Y	Fe	-7.302841	-7.302742	-7.302564	N/A	N/A	-7.582643	280	280	280	N/A	N/A	Fe ₂ YB ₂ + Fe _{4/3} Y _{2/3} AlB ₂ + Al ₈ Fe ₄ Y + ZrB ₂ + Al ₂ Y
Hf	Y	Sc	-7.546863	-7.546545	-7.546751	-7.607310	-7.565441	-7.664702	118	118	118	57	99	(Hf _{0.5} Sc _{0.5})B ₂ + AlSc ₂ + AlY ₂ + Al ₂ Y + (Hf _{0.75} Sc _{0.25})B ₂
Hf	Y	Y	-7.475354	-7.475647	-7.475840	-7.501517	-7.490518	-7.586148	111	110	110	84	95	(Y _{0.5} Hf _{0.5})B ₂ + (Hf _{0.75} Y _{0.25})B ₂ + AlY ₂ + Al ₂ Y
Hf	Y	Ti	-7.807369	-7.808226	-7.808355	-7.855302	-7.799439	-7.890685	83	82	82	35	91	(Hf _{0.5} Ti _{0.5})B ₂ + AlY ₂ + Al ₂ Y + Al ₃ Hf ₄
Hf	Y	Zr	-7.892315	-7.893150	-7.893206	-7.928312	-7.886949	-7.970350	78	77	77	42	83	(Zr _{0.5} Hf _{0.5})B ₂ + (Hf _{0.75} Zr _{0.25})B ₂ + AlY ₂ + Al ₂ Y + Al ₃ Zr ₄
Hf	Y	Hf	-8.077893	-8.078836	-8.078844	N/A	-8.066985	-8.121365	43	43	43	N/A	54	AlY ₂ + Al ₃ Hf ₄ + Al ₂ Y + HfB ₂
Hf	Y	V	-7.851240	-7.851715	-7.851641	-7.910754	-7.852033	-8.003090	152	151	151	92	151	(Hf _{0.75} Y _{0.25})B ₂ + Al ₂ Y + VB + HfB ₂
Hf	Y	Nb	-8.022649	-8.022381	-8.022378	-8.087976	-8.040483	-8.113719	91	91	91	26	73	AlY ₂ + (Hf _{0.75} Nb _{0.25})B ₂ + Al ₂ Y + NbB + HfB ₂
Hf	Y	Ta	-8.237877	-8.237638	-8.237669	-8.301323	-8.253681	-8.341291	103	104	104	40	88	(Hf _{0.75} Y _{0.25})B ₂ + Al ₂ Y + TaB + HfB ₂
Hf	Y	Cr	-7.774411	-7.774906	-7.774866	N/A	N/A	-7.994687	220	220	220	N/A	N/A	(Hf _{0.75} Y _{0.25})B ₂ + Al ₂ Y + CrB + HfB ₂
Hf	Y	Mo	-7.958311	-7.957136	-7.957067	N/A	N/A	-8.148864	191	192	192	N/A	N/A	Mo _{4/3} Y _{2/3} AlB ₂ + AlMo ₃ + AlY ₂ + Al ₂ Y + HfB ₂
Hf	Y	W	-8.170763	-8.169725	-8.169750	N/A	N/A	-8.377350	207	208	208	N/A	N/A	W _{4/3} Y _{2/3} AlB ₂ + (Hf _{0.75} Y _{0.25})B ₂ + Al ₂ Y + HfB ₂ + W
Hf	Y	Mn	-7.703307	-7.704222	-7.704218	N/A	N/A	-7.935389	232	231	231	N/A	N/A	AlY ₂ + Mn _{4/3} Y _{2/3} AlB ₂ + Al ₂ Y + Mn ₂ B + HfB ₂
Hf	Y	Fe	-7.550665	-7.550227	-7.550062	N/A	N/A	-7.832819	282	283	283	N/A	N/A	Fe ₂ YB ₂ + Fe _{4/3} Y _{2/3} AlB ₂ + Al ₂ Y + Al ₈ Fe ₄ Y + HfB ₂
V	Y	Sc	-7.365882	-7.366932	-7.366951	-7.375259	-7.317385	-7.424725	59	58	58	49	107	(Y _{0.75} Sc _{0.25})B ₂ + VYB ₄ + Al ₂ Y + VB + (Sc _{0.75} V _{0.25})B ₂
V	Y	Y	-7.269071	-7.269861	-7.269920	-7.220207	-7.223725	-7.333872	65	64	64	114	110	VYB ₄ + AlY ₂ + Al ₂ Y + VB
V	Y	Ti	-7.642570	-7.640859	-7.640953	-7.651600	-7.559192	-7.697914	55	57	57	46	139	(Ti _{0.75} V _{0.25})B ₂ + VYB ₄ + AlY ₂ + Al ₂ Y + VB
V	Y	Zr	-7.694125	-7.692470	-7.692590	-7.660303	-7.604555	-7.751146	57	59	59	91	147	V ₅ B ₆ + V ₃ B ₄ + (Zr _{0.75} Y _{0.25})B ₂ + Al ₂ Y + ZrB ₂
V	Y	Hf	-7.885411	-7.883616	-7.883807	-7.855893	-7.790400	-7.937366	52	54	54	81	147	V ₅ B ₆ + V ₃ B ₄ + (Hf _{0.75} Y _{0.25})B ₂ + Al ₂ Y + HfB ₂
V	Y	V	-7.696140	-7.694962	-7.694825	N/A	-7.629474	-7.729066	33	34	34	N/A	100	V ₂ B ₃ + VYB ₄ + YB ₄ + Al ₂ Y
V	Y	Nb	-7.841253	-7.839828	-7.839694	-7.842683	-7.768698	-7.850278	9	9	9	6	80	Nb _{4/3} Y _{2/3} V ₂ AlB ₆ + V ₃ B ₄ + (Nb _{0.75} V _{0.25}) ₃ B ₄ + (Nb _{0.5} Y _{0.5})B ₂ + Al ₂ Y
V	Y	Ta	-8.059462	-8.058377	-8.058349	-8.061210	-7.983317	-8.077166	18	13	13	10	88	(Ta _{0.5} V _{0.5}) ₃ B ₄ + (V _{0.75} Ta _{0.25}) ₃ B ₄ + Al ₃ Y + (Ta _{0.5} Y _{0.5})B ₂
V	Y	Cr	-7.627512	-7.629117	-7.628532	N/A	N/A	-7.738567	111	109	110	N/A	N/A	(Cr _{0.5} V _{0.5})B + (V _{0.75} Cr _{0.25}) ₃ B ₄ + Al ₃ Y + Cr ₂ V ₂ AlB ₆ + CrYB ₄
V	Y	Mo	-7.802736	-7.804450	-7.804855	N/A	N/A	-7.881081	78	77	76	N/A	N/A	V ₂ B ₃ + VB ₂ + YB ₄ + Al ₂ Y + Mo _{4/3} Y _{2/3} AlB ₂
V	Y	W	-8.017260	-8.018443	-8.018760	N/A	N/A	-8.117144	100	99	98	N/A	N/A	VB ₂ + YB ₄ + Al ₃ Y + (V _{0.5} W _{0.5})B
V	Y	Mn	-7.551413	-7.552959	-7.552964	N/A	N/A	-7.673790	122	121	121	N/A	N/A	MnYB ₄ + Mn _{4/3} Y _{2/3} V ₂ AlB ₆ + V ₃ B ₄ + Mn _{4/3} Y _{2/3} AlB ₂ + Al ₂ Y
V	Y	Fe	-7.403152	-7.407635	-7.407793	N/A	N/A	-7.571147	168	166	165	N/A	N/A	V ₃ B ₄ + Al ₈ Fe ₄ Y + V ₂ B ₃ + FeYB ₄ + Al ₂ Y
Nb	Y	Sc	-7.552689	-7.553389	-7.553582	-7.598546	-7.551821	-7.622704	70	69	69	24	71	AlY ₂ + (Nb _{0.5} Sc _{0.5}) ₄ AlB ₆ + Al ₂ Y + NbB + (Nb _{0.5} Sc _{0.5})B ₂
Nb	Y	Y	-7.473609	-7.474401	-7.474483	-7.473434	-7.462831	-7.514517	41	27	27	28	39	(Nb _{0.5} Y _{0.5})B ₂ + AlY ₂ + Al ₂ Y + NbB
Nb	Y	Ti	-7.810810	-7.809102	-7.809373	-7.836858	-7.776572	-7.855171	44	44	44	17	77	(Nb _{0.75} Ti _{0.25}) ₃ B ₄ + (Nb _{0.5} Y _{0.5})B ₂ + (Ti _{0.75} Nb _{0.25})B ₂ + AlY ₂ + Al ₂ Y
Nb	Y	Zr	-7.884743	-7.883386	-7.883606	-7.886840	-7.847267	-7.906293	22	22	21	18	58	(Zr _{0.75} Y _{0.25})B ₂ + (Zr _{0.75} Nb _{0.25})B ₂ + (Nb _{0.5} Y _{0.5})B ₂ + Al ₂ Y + NbB
Nb	Y	Hf	-8.073375	-8.071814	-8.072124	-8.074593	-8.030569	-8.094790	21	21	21	19	63	AlY ₂ + (Nb _{0.5} Y _{0.5})B ₂ + (Hf _{0.75} Nb _{0.25})B ₂ + Al ₂ Y + NbB

Nb	Y	V	-7.838409	-7.837212	-7.837155	-7.886289	-7.823805	-7.888134	50	49	50	0	63	$\text{Nb}_{4/3}\text{Y}_{2/3}\text{V}_2\text{AlB}_6 + \text{V}_3\text{B}_4 + (\text{Nb}_{0.75}\text{V}_{0.25})_3\text{B}_4 + (\text{Nb}_{0.5}\text{Y}_{0.5})\text{B}_2 + \text{Al}_2\text{Y}$
Nb	Y	Nb	-7.999381	-7.998852	-7.998789	N/A	-7.986994	-7.998481	-1	-2	-2	N/A	10	$(\text{Nb}_{0.83}\text{Y}_{0.17})_4\text{AlB}_6 + \text{Nb}_3\text{B}_4 + (\text{Nb}_{0.5}\text{Y}_{0.5})\text{B}_2 + \text{Al}_2\text{Y}$
Nb	Y	Ta	-8.215573	-8.214790	-8.214729	-8.246558	-8.198225	-8.244799	29	29	29	-3	45	$(\text{Nb}_{0.5}\text{Ta}_{0.5})_3\text{B}_4 + \text{Ta}_{4/3}\text{Y}_{2/3}\text{Nb}_2\text{AlB}_4 + (\text{Nb}_{0.5}\text{Y}_{0.5})\text{B}_2 + (\text{Ta}_{0.5}\text{Y}_{0.5})\text{B}_2 + \text{Al}_2\text{Y}$
Nb	Y	Cr	-7.764345	-7.765296	-7.765464	N/A	N/A	-7.887913	124	123	122	N/A	N/A	$\text{Cr}_{4/3}\text{Y}_{2/3}\text{Nb}_2\text{AlB}_6 + \text{Nb}_3\text{B}_4 + \text{Cr}_{4/3}\text{Y}_{2/3}\text{NbAlB}_4 + (\text{Nb}_{0.5}\text{Y}_{0.5})\text{B}_2 + \text{Al}_2\text{Y}$
Nb	Y	Mo	-7.939363	-7.943227	-7.943227	N/A	N/A	-8.049239	110	108	107	N/A	N/A	$\text{Nb}_{4/3}\text{Y}_{2/3}\text{NbAlB}_4 + \text{Mo}_{4/3}\text{Y}_{2/3}\text{NbAlB}_4$
Nb	Y	W	-8.150493	-8.153715	-8.154069	N/A	N/A	-8.268012	118	113	113	N/A	N/A	$\text{W}_{4/3}\text{Y}_{2/3}\text{NbAlB}_4 + \text{Al}_3\text{Nb} + (\text{Nb}_{0.5}\text{Y}_{0.5})\text{B}_2 + (\text{Nb}_{0.5}\text{W}_{0.5})\text{B}$
Nb	Y	Mn	-7.692348	-7.694193	-7.694458	N/A	N/A	-7.837635	145	144	144	N/A	N/A	$\text{Nb}_{4/3}\text{Y}_{2/3}\text{Nb}_2\text{AlB}_6 + \text{Nb}_3\text{B}_4 + \text{Mn}_{4/3}\text{Y}_{2/3}\text{NbAlB}_4 + (\text{Nb}_{0.5}\text{Y}_{0.5})\text{B}_2 + \text{Al}_2\text{Y}$
Nb	Y	Fe	-7.543639	-7.550250	-7.550681	N/A	N/A	-7.730015	186	180	180	N/A	N/A	$\text{Fe}_{4/3}\text{Y}_{2/3}\text{NbAlB}_4 + \text{Fe}_{4/3}\text{Y}_{2/3}\text{Nb}_2\text{AlB}_6 + \text{Nb}_3\text{B}_4 + (\text{Nb}_{0.5}\text{Y}_{0.5})\text{B}_2 + \text{Al}_8\text{Fe}_4\text{Y}$
Ta	Y	Sc	-7.843123	-7.843661	-7.843662	-7.888566	-7.837789	-7.923687	81	80	80	35	86	$\text{AlY}_2 + (\text{Sc}_{0.75}\text{Ta}_{0.25})\text{B}_2 + \text{TaB} + \text{Al}_2\text{Y} + (\text{Ta}_{0.5}\text{Sc}_{0.5})\text{B}_2$
Ta	Y	Y	-7.763468	-7.764162	-7.764255	-7.757872	-7.744563	-7.816261	53	31	31	38	51	$(\text{Y}_{0.5}\text{Ta}_{0.5})\text{B}_2 + \text{AlY}_2 + \text{Al}_2\text{Y} + \text{TaB}$
Ta	Y	Ti	-8.097173	-8.095592	-8.095847	-8.126390	-8.062851	-8.159657	62	61	61	31	94	$\text{AlY}_2 + (\text{Ti}_{0.75}\text{Ta}_{0.25})\text{B}_2 + (\text{Y}_{0.5}\text{Ta}_{0.5})\text{B}_2 + \text{Al}_2\text{Y} + \text{TaB}$
Ta	Y	Zr	-8.169013	-8.167657	-8.167883	-8.171117	-8.130887	-8.208462	39	39	39	35	76	$(\text{Zr}_{0.75}\text{Y}_{0.25})\text{B}_2 + (\text{Zr}_{0.75}\text{Ta}_{0.25})\text{B}_2 + (\text{Ta}_{0.5}\text{Y}_{0.5})\text{B}_2 + \text{Al}_2\text{Y} + \text{TaB}$
Ta	Y	Hf	-8.356215	-8.354816	-8.355063	-8.359048	-8.313387	-8.395957	40	39	39	35	81	$(\text{Hf}_{0.75}\text{Y}_{0.25})\text{B}_2 + (\text{Hf}_{0.75}\text{Ta}_{0.25})\text{B}_2 + (\text{Ta}_{0.5}\text{Y}_{0.5})\text{B}_2 + \text{Al}_2\text{Y} + \text{TaB}$
Ta	Y	V	-8.123730	-8.122443	-8.122432	-8.175617	-8.108113	-8.189819	66	61	61	8	75	$(\text{Ta}_{0.5}\text{V}_{0.5})_3\text{B}_4 + \text{Al}_3\text{Y} + (\text{Ta}_{0.5}\text{Y}_{0.5})\text{B}_2$
Ta	Y	Nb	-8.280732	-8.280360	-8.280191	-8.317351	-8.267362	-8.318905	38	34	34	-3	47	$(\text{Ta}_{0.5}\text{Nb}_{0.5})_3\text{B}_4 + \text{Al}_3\text{Y} + (\text{Ta}_{0.5}\text{Y}_{0.5})\text{B}_2$
Ta	Y	Ta	-8.494992	-8.494362	-8.494108	N/A	-8.476222	-8.513408	18	11	11	N/A	29	$(\text{Ta}_{0.5}\text{Y}_{0.5})\text{B}_2 + \text{Ta}_3\text{B}_4 + \text{Al}_3\text{Y}$
Ta	Y	Cr	-8.050212	-8.051078	-8.051260	N/A	N/A	-8.179726	130	128	128	N/A	N/A	$\text{Al}_3\text{Y} + \text{Ta}_3\text{B}_4 + \text{Cr}_{4/3}\text{Y}_{2/3}\text{TaAlB}_4 + \text{CrYB}_4$
Ta	Y	Mo	-8.220323	-8.223004	-8.223313	N/A	N/A	-8.343989	124	117	116	N/A	N/A	$\text{Mo}_{4/3}\text{Y}_{2/3}\text{TaAlB}_4 + \text{Al}_{22}\text{Mo}_5 + (\text{Ta}_{0.5}\text{Y}_{0.5})\text{B}_2 + \text{Al}_2\text{Y} + (\text{Ta}_{0.75}\text{Mo}_{0.25})\text{B}$
Ta	Y	W	-8.428162	-8.430329	-8.430654	N/A	N/A	-8.561175	133	124	124	N/A	N/A	$(\text{Ta}_{0.5}\text{Y}_{0.5})\text{B}_2 + \text{Al}_3\text{Y} + \text{W}_{4/3}\text{Y}_{2/3}\text{AlB}_2 + \text{Al}_5\text{W} + (\text{Ta}_{0.5}\text{W}_{0.5})\text{B}$
Ta	Y	Mn	-7.978908	-7.980488	-7.980385	N/A	N/A	-8.129064	150	147	147	N/A	N/A	$\text{Ta}_3\text{B}_4 + \text{Mn}_{4/3}\text{Y}_{2/3}\text{TaAlB}_4 + \text{Al}_3\text{Y} + (\text{Ta}_{0.5}\text{Y}_{0.5})\text{B}_2$
Ta	Y	Fe	-7.828539	-7.834857	-7.835106	N/A	N/A	-8.023700	195	186	186	N/A	N/A	$\text{Fe}_{4/3}\text{Y}_{2/3}\text{Ta}_2\text{AlB}_6 + \text{Ta}_3\text{B}_4 + \text{Fe}_{4/3}\text{Y}_{2/3}\text{TaAlB}_4 + \text{Al}_8\text{Fe}_4\text{Y} + (\text{Ta}_{0.5}\text{Y}_{0.5})\text{B}_2$
Cr	Y	Sc	-7.379803	-7.379339	-7.379431	-7.335226	-7.290964	-7.409945	30	31	31	75	119	$\text{Cr}_4\text{AlB}_4 + \text{CrYB}_4 + \text{Al}_2\text{Y} + \text{CrB} + \text{ScB}_2$
Cr	Y	Y	-7.279934	-7.279424	-7.279451	-7.176842	-7.205112	-7.360571	81	81	81	184	155	$\text{CrYB}_4 + \text{CrB} + \text{AlY}_2 + \text{Al}_2\text{Y}$
Cr	Y	Ti	-7.652442	-7.652035	-7.651976	-7.611279	-7.523991	-7.686524	34	34	35	75	163	$\text{CrYB}_4 + \text{CrB} + \text{Cr}_4\text{AlB}_4 + \text{Al}_2\text{Y} + \text{TiB}_2$
Cr	Y	Zr	-7.698901	-7.698184	-7.698150	-7.607861	-7.573575	-7.742542	44	44	44	135	169	$\text{CrYB}_4 + \text{CrB} + \text{Cr}_4\text{AlB}_4 + \text{Al}_2\text{Y} + \text{ZrB}_2$
Cr	Y	Hf	-7.890582	-7.890059	-7.890092	-7.804244	-7.755168	-7.930174	40	40	40	126	175	$\text{Cr}_4\text{AlB}_4 + \text{CrYB}_4 + \text{Al}_2\text{Y} + \text{CrB} + \text{HfB}_2$
Cr	Y	V	-7.712011	-7.711783	-7.711712	-7.699064	-7.593162	-7.737104	25	25	25	38	144	$(\text{Cr}_{0.5}\text{V}_{0.5})\text{B} + (\text{V}_{0.75}\text{Cr}_{0.25})_3\text{B}_4 + \text{Cr}_2\text{V}_2\text{AlB}_6 + \text{Al}_3\text{Y} + \text{CrYB}_4$
Cr	Y	Nb	-7.850223	-7.849679	-7.849461	-7.796425	-7.727742	-7.845032	-5	-5	-4	49	117	$\text{Cr}_{4/3}\text{Y}_{2/3}\text{Nb}_2\text{AlB}_6 + \text{Cr}_4\text{AlB}_4 + \text{CrYB}_4 + \text{Al}_2\text{Y} + \text{CrB}$
Cr	Y	Ta	-8.068499	-8.068033	-8.067896	-8.014138	-7.940103	-8.057921	-11	-10	-10	44	118	$\text{Ta}_3\text{B}_4 + \text{Cr}_4\text{AlB}_4 + \text{Cr}_{4/3}\text{Y}_{2/3}\text{Ta}_2\text{AlB}_6 + \text{CrYB}_4 + \text{Al}_2\text{Y}$
Cr	Y	Cr	-7.650653	-7.653112	-7.653316	N/A	N/A	-7.713344	63	60	60	N/A	N/A	$\text{CrYB}_4 + \text{Cr}_2\text{AlB}_2 + \text{Al}_3\text{Y} + \text{Cr}_4\text{AlB}_4$
Cr	Y	Mo	-7.819332	-7.823708	-7.824069	N/A	N/A	-7.873474	54	50	49	N/A	N/A	$(\text{Cr}_{0.75}\text{Mo}_{0.25})\text{B} + \text{Cr}_4\text{AlB}_4 + \text{CrYB}_4 + \text{Mo}_{4/3}\text{Y}_{2/3}\text{AlB}_2 + \text{MoAlB}$
Cr	Y	W	-8.032502	-8.035967	-8.036481	N/A	N/A	-8.094149	62	58	58	N/A	N/A	$(\text{Cr}_{0.75}\text{W}_{0.25})\text{B} + \text{Al}_3\text{Y} + \text{W}_{4/3}\text{Y}_{2/3}\text{AlB}_2 + \text{Al}_5\text{W} + \text{CrYB}_4$
Cr	Y	Mn	-7.567415	-7.571036	-7.571073	N/A	N/A	-7.678854	111	108	108	N/A	N/A	$\text{CrYB}_4 + (\text{Mn}_{0.67}\text{Cr}_{0.33})_2\text{AlB}_2 + (\text{Cr}_{0.67}\text{Mn}_{0.33})_2\text{AlB}_2 + \text{Mn}_{4/3}\text{Y}_{2/3}\text{AlB}_2$
Cr	Y	Fe	-7.424234	-7.431839	-7.431864	N/A	N/A	-7.565461	141	134	134	N/A	N/A	$\text{AlMo}_3 + (\text{Fe}_{0.67}\text{Cr}_{0.33})_2\text{AlB}_2 + \text{Al}_8\text{Fe}_4\text{Y} + \text{CrB} + (\text{Cr}_{0.67}\text{Fe}_{0.33})_2\text{AlB}_2$
Mo	Y	Sc	-7.626432	-7.626608	-7.626537	-7.614511	-7.566557	-7.642490	16	16	16	28	76	$\text{AlMo}_3 + \text{AlY}_2 + \text{Al}_2\text{Y} + \text{Mo}_{4/3}\text{Y}_{2/3}\text{AlB}_2 + (\text{Sc}_{0.75}\text{Mo}_{0.25})\text{B}_2$
Mo	Y	Y	-7.536588	-7.536641	-7.536599	-7.474263	-7.481368	-7.542890	6	6	6	69	62	$\text{AlY}_2 + \text{Mo}_{4/3}\text{Y}_{2/3}\text{AlB}_2 + \text{MoYB}_4 + \text{Al}_2\text{Y}$
Mo	Y	Ti	-7.880725	-7.879292	-7.879287	-7.855394	-7.786695	-7.901613	21	22	22	46	115	$\text{Mo}_{4/3}\text{Y}_{2/3}\text{AlB}_2 + \text{TiB}_2$
Mo	Y	Zr	-7.942598	-7.941348	-7.941285	-7.883391	-7.844174	-7.957631	15	16	16	74	113	$\text{Mo}_{4/3}\text{Y}_{2/3}\text{AlB}_2 + \text{ZrB}_2$
Mo	Y	Hf	-8.132760	-8.131441	-8.131285	-8.074291	-8.026078	-8.145263	13	14	14	71	119	$\text{Mo}_{4/3}\text{Y}_{2/3}\text{AlB}_2 + \text{HfB}_2$
Mo	Y	V	-7.914972	-7.917271	-7.917066	-7.915807	-7.842002	-7.931464	16	14	14	16	89	$\text{VB}_2 + \text{Mo}_{4/3}\text{Y}_{2/3}\text{AlB}_2$
Mo	Y	Nb	-8.065859	-8.067825	-8.067677	-8.038740	-7.984569	-8.058281	-8	-10	-9	20	74	$\text{Mo}_{4/3}\text{Y}_{2/3}\text{Nb}_2\text{AlB}_6 + \text{Mo}_{4/3}\text{Y}_{2/3}\text{AlB}_2$
Mo	Y	Ta	-8.282300	-8.283928	-8.284007	-8.251634	-8.193232	-8.273699	-9	-16	-16	16	75	$(\text{Mo}_{0.5}\text{Ta}_{0.5})\text{B} + \text{Al}_{22}\text{Mo}_5 + \text{Mo}_{4/3}\text{Y}_{2/3}\text{AlB}_2 + \text{MoAlB} + (\text{Ta}_{0.5}\text{Y}_{0.5})\text{B}_2$
Mo	Y	Cr	-7.845473	-7.848289	-7.848121	N/A	N/A	-7.923927	78	76	76	N/A	N/A	$(\text{Cr}_{0.75}\text{Mo}_{0.25})\text{B} + (\text{Cr}_{0.5}\text{Mo}_{0.5})\text{B} + \text{CrYB}_4 + \text{Mo}_{4/3}\text{Y}_{2/3}\text{AlB}_2 + \text{MoAlB}$
Mo	Y	Mo	-8.019440	-8.023692	-8.023268	N/A	N/A	-8.054191	35	30	31	N/A	N/A	$\text{MoAlB} + \text{Mo}_4\text{AlB}_4 + \text{Mo}_{4/3}\text{Y}_{2/3}\text{AlB}_2 + \text{MoYB}_4$

Mo	Y	W	-8.228242	-8.233161	-8.233034	N/A	N/A	-8.298650	70	65	66	N/A	N/A	(Mo _{0.5} W _{0.5})AlB + (Mo _{0.5} W _{0.5})B + MoYB ₄ + W _{4/3} Y _{2/3} AlB ₂ + Mo _{4/3} Y _{2/3} AlB ₂
Mo	Y	Mn	-7.767068	-7.769499	-7.769221	N/A	N/A	-7.850702	84	81	81	N/A	N/A	(Mo _{0.67} Mn _{0.33}) ₂ AlB ₂ + MnYB ₄ + Mo _{4/3} Y _{2/3} AlB ₂
Mo	Y	Fe	-7.620603	-7.628546	-7.628900	N/A	N/A	-7.740591	120	112	112	N/A	N/A	Mo ₄ AlB ₄ + FeYB ₄ + MoAlB + Fe ₂ AlB ₂ + Al ₈ Fe ₄ Y
W	Y	Sc	-7.933722	-7.933300	-7.933216	-7.913608	-7.865318	-7.951307	18	18	18	38	86	W _{4/3} Y _{2/3} AlB ₂ + ScW ₂ B ₄ + (Sc _{0.75} W _{0.25})B ₂ + WY ₃ B ₇ + Al ₂ Y
W	Y	Y	-7.843132	-7.842958	-7.842890	-7.769875	-7.777853	-7.854321	11	11	11	84	76	W _{4/3} Y _{2/3} AlB ₂ + WY ₃ B ₇ + YB ₄ + Al ₂ Y
W	Y	Ti	-8.179454	-8.177645	-8.177628	-8.149152	-8.080910	-8.199326	20	22	22	50	118	W _{4/3} Y _{2/3} AlB ₂ + TiB ₂
W	Y	Zr	-8.240165	-8.238887	-8.238844	-8.174555	-8.135985	-8.255345	15	16	17	81	119	W _{4/3} Y _{2/3} AlB ₂ + ZrB ₂
W	Y	Hf	-8.428822	-8.427459	-8.427323	-8.363664	-8.316154	-8.442977	14	16	16	79	127	W _{4/3} Y _{2/3} AlB ₂ + HfB ₂
W	Y	V	-8.207372	-8.209273	-8.209230	-8.206109	-8.131687	-8.237754	30	28	29	32	106	W _{4/3} Y _{2/3} AlB ₂ + YB ₄ + Al ₅ Y + Al ₅ W + (V _{0.5} W _{0.5})B
W	Y	Nb	-8.354067	-8.355921	-8.355813	-8.324246	-8.270643	-8.350011	-4	-6	-6	26	79	W _{4/3} Y _{2/3} Nb ₂ AlB ₆ + W _{4/3} Y _{2/3} AlB ₂
W	Y	Ta	-8.568227	-8.568919	-8.568996	-8.533268	-8.475749	-8.567537	-1	-6	-6	29	87	(Ta _{0.5} Y _{0.5})B ₂ + (W _{0.75} Ta _{0.25})B + W _{4/3} Y _{2/3} AlB ₂ + Al ₅ W + (Ta _{0.5} W _{0.5})B
W	Y	Cr	-8.135752	-8.138586	-8.138405	N/A	N/A	-8.218156	82	80	80	N/A	N/A	(Cr _{0.5} W _{0.5})AlB + W _{4/3} Y _{2/3} AlB ₂ + (W _{0.75} Cr _{0.25})B + Al ₅ W + CrYB ₄
W	Y	Mo	-8.302405	-8.310940	-8.307035	N/A	N/A	-8.371855	69	61	65	N/A	N/A	(Mo _{0.5} W _{0.5})AlB + (Mo _{0.5} W _{0.5})B + MoYB ₄ + YB ₄ + W _{4/3} Y _{2/3} AlB ₂
W	Y	W	-8.506133	-8.514587	-8.512159	N/A	N/A	-8.568195	62	54	56	N/A	N/A	W _{4/3} Y _{2/3} AlB ₂ + WAlB + WB + YB ₄
W	Y	Mn	-8.058531	-8.061079	-8.060723	N/A	N/A	-8.144823	86	84	84	N/A	N/A	(W _{0.75} Mn _{0.25})B + W _{4/3} Y _{2/3} AlB ₂ + Mn ₂ AlB ₂ + MnYB ₄ + WAlB
W	Y	Fe	-7.909766	-7.921218	-7.921515	N/A	N/A	-8.038432	129	117	117	N/A	N/A	Al ₈ Fe ₄ Y + WAlB + Fe ₂ AlB ₂ + FeW ₂ B ₂ + FeYB ₄
Mn	Y	Sc	-7.318741	-7.318369	-7.318372	-7.235493	-7.201058	-7.338505	20	20	20	103	137	Mn _{4/3} Y _{2/3} AlB ₂ + ScB ₂
Mn	Y	Y	-7.214446	-7.213567	-7.213561	-7.084810	-7.122365	-7.269563	55	56	56	185	147	Mn _{4/3} Y _{2/3} AlB ₂ + MnY ₃ B ₇ + MnYB ₄ + Al ₂ Y
Mn	Y	Ti	-7.591600	-7.591285	-7.591349	-7.511201	-7.428224	-7.615084	23	24	24	104	187	Mn _{4/3} Y _{2/3} AlB ₂ + TiB ₂
Mn	Y	Zr	-7.633493	-7.632634	-7.632661	-7.509791	-7.485084	-7.671102	38	38	38	161	186	Mn _{4/3} Y _{2/3} AlB ₂ + ZrB ₂
Mn	Y	Hf	-7.825821	-7.825097	-7.825214	-7.704440	-7.664241	-7.858734	33	34	34	154	194	Mn _{4/3} Y _{2/3} AlB ₂ + HfB ₂
Mn	Y	V	-7.652540	-7.653532	-7.653921	-7.605186	-7.502184	-7.653239	1	0	-1	48	151	Mn _{4/3} Y _{2/3} V ₂ AlB ₆ + Mn _{4/3} Y _{2/3} AlB ₂
Mn	Y	Nb	-7.783286	-7.784060	-7.784588	-7.698149	-7.637735	-7.775621	-8	-8	-9	77	138	Mn _{4/3} Y _{2/3} Nb ₂ AlB ₆ + Mn _{4/3} Y _{2/3} AlB ₂
Mn	Y	Ta	-8.000950	-8.001598	-8.002074	-7.914644	-7.845488	-7.987120	-14	-14	-15	72	142	Mn _{4/3} Y _{2/3} Ta ₂ AlB ₆ + Mn _{4/3} Y _{2/3} AlB ₂
Mn	Y	Cr	-7.596890	-7.604283	-7.604325	N/A	N/A	-7.657866	61	54	54	N/A	N/A	CrYB ₄ + (Mn _{0.67} Cr _{0.33}) ₂ AlB ₂ + Mn _{4/3} Y _{2/3} AlB ₂
Mn	Y	Mo	-7.756853	-7.768644	-7.768291	N/A	N/A	-7.780143	23	11	12	N/A	N/A	(Mn _{0.67} Mo _{0.33}) ₂ AlB ₂ + (Mo _{0.67} Mn _{0.33}) ₂ AlB ₂ + MnYB ₄ + Mo _{4/3} Y _{2/3} AlB ₂
Mn	Y	W	-7.965963	-7.980349	-7.979829	N/A	N/A	-8.000890	35	21	21	N/A	N/A	(W _{0.75} Mn _{0.25})B + W _{4/3} Y _{2/3} AlB ₂ + Mn ₂ AlB ₂ + MnYB ₄ + WAlB
Mn	Y	Mn	-7.506052	-7.511106	-7.511153	N/A	N/A	-7.566963	61	56	56	N/A	N/A	Mn _{4/3} Y _{2/3} AlB ₂ + Mn ₂ AlB ₂ + MnYB ₄
Mn	Y	Fe	-7.353986	-7.365672	-7.366191	N/A	N/A	-7.478808	125	113	113	N/A	N/A	(Fe _{0.67} Mn _{0.33}) ₂ AlB ₂ + Fe _{4/3} Y _{2/3} AlB ₂ + MnYB ₄ + (Mn _{0.67} Fe _{0.33}) ₂ AlB ₂
Fe	Y	Sc	-7.180952	-7.181727	-7.181536	-7.059520	-7.044799	-7.198395	17	17	17	139	154	Fe _{4/3} Y _{2/3} AlB ₂ + ScB ₂
Fe	Y	Y	-7.076109	-7.076425	-7.076206	-6.919441	-6.976362	-7.130330	54	54	54	211	154	FeY ₃ B ₇ + Fe ₂ YB ₂ + FeYB ₄ + Al ₂ Y
Fe	Y	Ti	-7.447460	-7.448651	-7.448324	-7.333645	-7.265338	-7.474974	28	26	27	141	210	Fe _{4/3} Y _{2/3} AlB ₂ + TiB ₂
Fe	Y	Zr	-7.482595	-7.482332	-7.482070	-7.329810	-7.321503	-7.530992	48	49	49	201	209	Fe _{4/3} Y _{2/3} AlB ₂ + ZrB ₂
Fe	Y	Hf	-7.677073	-7.676592	-7.676394	-7.523913	-7.501777	-7.718624	42	42	42	195	217	Fe _{4/3} Y _{2/3} AlB ₂ + HfB ₂
Fe	Y	V	-7.512469	-7.520982	-7.521087	-7.432717	-7.338460	-7.511514	-1	-9	-10	79	173	Fe _{4/3} Y _{2/3} V ₂ AlB ₆ + Fe _{4/3} Y _{2/3} AlB ₂
Fe	Y	Nb	-7.635186	-7.640766	-7.640766	-7.517172	-7.473091	-7.630984	-4	-10	-10	114	158	Fe _{4/3} Y _{2/3} Nb ₂ AlB ₆ + Fe _{4/3} Y _{2/3} AlB ₂
Fe	Y	Ta	-7.854509	-7.858762	-7.858659	-7.733161	-7.683564	-7.843366	-11	-15	-15	110	160	Fe _{4/3} Y _{2/3} Ta ₂ AlB ₆ + Fe _{4/3} Y _{2/3} AlB ₂
Fe	Y	Cr	-7.442032	-7.445507	-7.445484	N/A	N/A	-7.507165	65	62	62	N/A	N/A	CrYB ₄ + Fe _{4/3} Y _{2/3} AlB ₂ + (Fe _{0.67} Cr _{0.33}) ₂ AlB ₂
Fe	Y	Mo	-7.604560	-7.609470	-7.609246	N/A	N/A	-7.634249	30	25	25	N/A	N/A	Mo ₄ AlB ₄ + FeYB ₄ + MoAlB + Fe ₂ AlB ₂ + Al ₈ Fe ₄ Y
Fe	Y	W	-7.817473	-7.822677	-7.822623	N/A	N/A	-7.858453	41	36	36	N/A	N/A	Al ₈ Fe ₄ Y + WAlB + Fe ₂ AlB ₂ + FeW ₂ B ₂ + FeYB ₄
Fe	Y	Mn	-7.343424	-7.353924	-7.352318	N/A	N/A	-7.442738	99	89	90	N/A	N/A	(Fe _{0.67} Mn _{0.33}) ₂ AlB ₂ + Fe _{4/3} Y _{2/3} AlB ₂ + MnYB ₄
Fe	Y	Fe	-7.184838	-7.198572	-7.198545	N/A	N/A	-7.314620	130	116	116	N/A	N/A	Fe _{4/3} Y _{2/3} AlB ₂ + Fe ₂ AlB ₂ + FeYB ₄

Table S4. Calculated energy (E) and stability at 2000 K (ΔG_{cp}^{s-MAB} , $\Delta G_{cp}^{partial\ disorder}$, $\Delta G_{cp}^{disorder}$) for M2 = Sc in s-MAB, s-MAB with disorder, and MAB with disorder for 416 MAB phases along with corresponding energy for their competing phases and identified set of most competing phases. Phases modelled with solid solution disorder have a contribution from configurational entropy evaluated at 2000 K. Competing phases in bold highlight when a MAB phase is part of the set of most competing phases.

M1	M2	M3	Energy (eV/atom)					ΔG_{cp} (meV/atom)					Set of most competing phases	
			s-MAB (no. 191)	s-MAB (no. 194)	s-MAB (no. 166)	s-MAB disorder	MAB disorder	Competing phases	s-MAB (no. 191)	s-MAB (no. 194)	s-MAB (no. 166)	s-MAB partial disorder		MAB disorder
Sc	Sc	Y	N/A	N/A	N/A	N/A	-6.961111	-7.004262	N/A	N/A	N/A	N/A	43	(Sc _{0.75} Y _{0.25})B ₂ + (Y _{0.75} Sc _{0.25})B ₂ + AlY ₂ + Al ₂ Y
Sc	Sc	Ti	N/A	N/A	N/A	N/A	-7.449757	-7.477179	N/A	N/A	N/A	N/A	27	(Sc _{0.5} Ti _{0.5})B ₂ + (Ti _{0.75} Sc _{0.25})B ₂ + AlSc
Sc	Sc	Zr	N/A	N/A	N/A	N/A	-7.551725	-7.575314	N/A	N/A	N/A	N/A	24	(Sc _{0.5} Zr _{0.5})B ₂ + AlSc + (Zr _{0.75} Sc _{0.25})B ₂
Sc	Sc	Hf	N/A	N/A	N/A	N/A	-7.823775	-7.854524	N/A	N/A	N/A	N/A	31	(Sc _{0.5} Hf _{0.5})B ₂ + AlSc + (Hf _{0.75} Sc _{0.25})B ₂
Sc	Sc	V	N/A	N/A	N/A	N/A	-7.562869	-7.587631	N/A	N/A	N/A	N/A	25	(Sc _{0.5} V _{0.5})B ₂ + Al ₃ Sc + VB + (Sc _{0.75} V _{0.25})B ₂
Sc	Sc	Nb	N/A	N/A	N/A	N/A	-7.813008	-7.804826	N/A	N/A	N/A	N/A	-8	(Nb _{0.44} Sc _{0.56}) ₃ AlB ₄ + Al ₂ Sc + NbB + (Sc _{0.5} Nb _{0.5})B ₂
Sc	Sc	Ta	N/A	N/A	N/A	N/A	-8.132857	-8.129230	N/A	N/A	N/A	N/A	-4	(Sc _{0.5} Ta _{0.5})B ₂ + Al ₂ Sc + TaB + (Sc _{0.75} Ta _{0.25})B ₂
Y	Sc	Sc	-6.954710	-6.932915	-6.922251	-6.947619	-6.995361	-7.042995	88	110	121	95	48	(Sc _{0.75} Y _{0.25})B ₂ + AlY ₂ + Al ₂ Y + ScB ₂
Y	Sc	Y	-6.847802	-6.813955	-6.814404	N/A	-6.910511	-6.922834	75	109	108	N/A	12	(Y _{0.75} Sc _{0.25})B ₂ + AlY ₂ + YB ₂ + Al ₂ Y
Y	Sc	Ti	-7.343251	-7.342990	-7.343036	-7.295912	-7.337480	-7.462532	119	120	119	167	125	(Ti _{0.75} Sc _{0.25})B ₂ + AlY ₂ + YB ₂ + Al ₂ Y
Y	Sc	Zr	-7.457257	-7.426810	-7.426469	-7.433862	-7.472078	-7.558886	102	132	132	125	87	(Y _{0.75} Zr _{0.25})B ₂ + (Zr _{0.75} Sc _{0.25})B ₂ + (Sc _{0.5} Zr _{0.5})B ₂ + AlY ₂ + Al ₂ Y
Y	Sc	Hf	-7.730885	-7.702649	-7.700686	-7.696334	-7.732977	-7.836474	106	134	136	140	103	AlY ₂ + YB ₂ + Al ₂ Y + (Hf _{0.75} Sc _{0.25})B ₂
Y	Sc	V	-7.406528	-7.359284	-7.406678	-7.375762	-7.430327	-7.541972	135	183	135	166	112	(Y _{0.75} Sc _{0.25})B ₂ + VYB ₄ + Al ₂ Y + VB + (Sc _{0.75} V _{0.25})B ₂
Y	Sc	Nb	-7.635600	-7.602777	-7.602477	-7.653580	-7.706308	-7.747035	111	144	145	93	41	(Nb _{0.5} Y _{0.5})B ₂ + AlY ₂ + Al ₂ Y + NbB + (Sc _{0.5} Nb _{0.5})B ₂
Y	Sc	Ta	-7.947299	-7.920888	-7.913456	-7.964996	-8.018811	-8.070433	123	150	157	105	52	(Ta _{0.5} Y _{0.5})B ₂ + (Y _{0.75} Ta _{0.25})B ₂ + TaB + Al ₂ Y + (Sc _{0.5} Ta _{0.5})B ₂
Y	Sc	Cr	-7.291311	-7.305327	-7.253455	N/A	N/A	-7.549475	258	244	296	N/A	N/A	Cr ₄ AlB ₄ + CrYB ₄ + Al ₂ Y + CrB + ScB ₂
Y	Sc	Mo	-7.539379	-7.500055	-7.499987	N/A	N/A	-7.776171	237	276	276	N/A	N/A	MoYB ₄ + AlY ₂ + Al ₂ Y + CrB + ScB ₂ + (Sc _{0.75} Mo _{0.25})B ₂
Y	Sc	W	-7.835484	-7.835823	-7.799169	N/A	N/A	-8.098787	263	263	300	N/A	N/A	W _{4/3} Y _{2/3} AlB ₂ + ScW ₂ B ₄ + (Sc _{0.75} W _{0.25})B ₂ + WY ₃ B ₇ + YB ₄
Y	Sc	Mn	-7.171931	-7.172022	-7.136390	N/A	N/A	-7.461020	289	289	325	N/A	N/A	MnYB ₄ + Mn _{4/3} Y _{2/3} AlB ₂ + ScB ₂
Y	Sc	Fe	-6.953827	-6.916451	-6.918605	N/A	N/A	-7.305818	352	389	387	N/A	N/A	FeYB ₄ + Fe _{4/3} Y _{2/3} AlB ₂ + ScB ₂
Ti	Sc	Sc	-7.277836	-7.115522	-7.278077	-7.306270	-7.318607	-7.340453	63	225	62	34	22	(Sc _{0.5} Ti _{0.5})B ₂ + AlSc + (Sc _{0.75} Ti _{0.25})B ₂
Ti	Sc	Y	-7.136155	-7.136228	-7.135968	-7.131032	-7.176495	-7.282633	146	146	147	152	106	(Y _{0.75} Sc _{0.25})B ₂ + (Ti _{0.75} Sc _{0.25})B ₂ + AlY ₂ + YB ₂ + Al ₂ Y
Ti	Sc	Ti	-7.689794	-7.689787	-7.689897	N/A	-7.714300	-7.704607	15	15	15	N/A	-10	(Ti _{0.78} Sc _{0.22}) ₃ AlB ₄ + TiB ₂
Ti	Sc	Zr	-7.769420	-7.769467	-7.769399	-7.774606	-7.787447	-7.808650	39	39	39	34	21	(Ti _{0.83} Sc _{0.17}) ₄ AlB ₆ + (Zr _{0.83} Sc _{0.17}) ₄ AlB ₆
Ti	Sc	Hf	-8.047620	-8.047704	-8.047682	-8.056471	-8.065810	-8.078671	31	31	31	22	13	(Ti _{0.83} Sc _{0.17}) ₄ AlB ₆ + (Hf _{0.83} Sc _{0.17}) ₄ AlB ₆
Ti	Sc	V	-7.755064	-7.754317	-7.754905	-7.824846	-7.816259	-7.853294	98	99	98	28	37	(Ti _{0.75} V _{0.25})B ₂ + (Sc _{0.5} V _{0.5})B ₂ + (Ti _{0.75} Sc _{0.25})B ₂ + Al ₃ Sc + VB
Ti	Sc	Nb	-7.948483	-7.947645	-7.948144	-8.011361	-8.032122	-8.039345	91	92	91	28	7	(Nb _{0.75} Ti _{0.25}) ₅ B ₆ + (Ti _{0.75} Nb _{0.25})B ₂ + (Nb _{0.5} Sc _{0.5}) ₄ AlB ₆ + Al ₃ Nb + TiB ₂
Ti	Sc	Ta	-8.256338	-8.255482	-8.255748	-8.327029	-8.351716	-8.365618	109	110	110	39	14	(Ta _{0.75} Ti _{0.25}) ₅ B ₆ + TaB + (Ti _{0.75} Ta _{0.25})B ₂ + (Sc _{0.5} Ta _{0.5})B ₂ + Al ₃ Sc
Ti	Sc	Cr	-7.340683	-7.645948	-7.645994	N/A	N/A	-7.841646	501	196	196	N/A	N/A	(Sc _{0.5} Ti _{0.5})B ₂ + Cr ₂ AlB ₂ + (Ti _{0.75} Sc _{0.25})B ₂
Ti	Sc	Mo	-7.868020	-7.869157	-7.868367	N/A	N/A	-8.066297	198	197	198	N/A	N/A	(Mo _{0.75} Ti _{0.25}) ₅ B ₆ + (Ti _{0.75} Sc _{0.25})B ₂ + Mo ₄ AlB ₄ + (Sc _{0.75} Mo _{0.25})B ₂ + MoAlB
Ti	Sc	W	-8.156868	-8.157755	-8.157151	N/A	N/A	-8.392217	235	234	235	N/A	N/A	ScW ₂ B ₄ + (Sc _{0.75} Ti _{0.25})B ₂ + (Sc _{0.75} W _{0.25})B ₂ + WAlB + TiB ₂
Ti	Sc	Mn	-7.527415	-7.526433	-7.526553	N/A	N/A	-7.754602	227	228	228	N/A	N/A	(Sc _{0.5} Ti _{0.5})B ₂ + (Ti _{0.75} Sc _{0.25})B ₂ + Mn ₂ AlB ₂
Ti	Sc	Fe	-7.307390	-7.308467	-7.308139	N/A	N/A	-7.597176	290	289	289	N/A	N/A	(Sc _{0.5} Ti _{0.5})B ₂ + (Ti _{0.75} Sc _{0.25})B ₂ + Fe ₂ AlB ₂

Zr	Sc	Sc	-7.318659	-7.318412	-7.318092	-7.371909	-7.392108	-7.411914	93	94	94	40	20	(Sc _{0.5} Zr _{0.5})B ₂ + AlSc + (Sc _{0.75} Zr _{0.25})B ₂
Zr	Sc	Y	-7.198933	-7.198593	-7.198456	-7.244488	-7.279362	-7.349211	150	151	151	105	70	(Y _{0.75} Zr _{0.25})B ₂ + (Zr _{0.75} Sc _{0.25})B ₂ + (Sc _{0.5} Zr _{0.5})B ₂ + AlY ₂ + Al ₂ Y
Zr	Sc	Ti	-7.713397	-7.713480	-7.713579	-7.747144	-7.757620	-7.777200	64	64	64	30	20	(Ti _{0.83} Sc _{0.17}) ₄ AlB ₆ + (Zr _{0.83} Sc _{0.17}) ₄ AlB ₆
Zr	Sc	Zr	-7.819353	-7.819367	-7.819606	N/A	-7.871549	-7.860100	41	41	40	N/A	-11	Al ₃ Zr ₂ + Al ₃ Zr ₄ + ZrB ₂ + (Zr _{0.75} Sc _{0.25})B ₂
Zr	Sc	Hf	-8.093540	-8.093585	-8.093846	-8.125684	-8.141210	-8.152648	59	59	59	27	11	Al ₃ Zr ₂ + AlSc + (Hf _{0.5} Zr _{0.5})B ₂ + (Hf _{0.75} Zr _{0.25})B ₂ + Al ₃ Zr ₄
Zr	Sc	V	-7.762783	-7.761206	-7.761944	-7.812792	-7.834458	-7.911476	149	150	150	99	77	(Zr _{0.75} Sc _{0.25})B ₂ + V ₃ B ₄ + Al ₃ Zr + Al ₃ Sc
Zr	Sc	Nb	-7.972131	-7.974546	-7.975295	-8.052148	-8.086105	-8.097558	125	123	122	45	11	NbB + (Zr _{0.75} Sc _{0.25})B ₂ + (Zr _{0.75} Nb _{0.25})B ₂ + Al ₃ Nb + (Nb _{0.5} Sc _{0.5})B ₂
Zr	Sc	Ta	-8.278853	-8.280834	-8.281282	-8.360777	-8.399750	-8.419001	140	138	138	58	19	(Zr _{0.75} Sc _{0.25})B ₂ + Al ₃ Zr + (Zr _{0.75} Ta _{0.25})B ₂ + (Ta _{0.5} Sc _{0.5})B ₂ + TaB
Zr	Sc	Cr	-7.642787	-7.643300	-7.643439	N/A	N/A	-7.907070	264	264	264	N/A	N/A	(Zr _{0.75} Sc _{0.25})B ₂ + Cr ₂ AlB ₂ + (Zr _{0.5} Sc _{0.5})B ₂
Zr	Sc	Mo	-7.875843	-7.880353	-7.879598	N/A	N/A	-8.129116	253	249	250	N/A	N/A	Al ₃ Mo ₃ + (Zr _{0.75} Sc _{0.25})B ₂ + Mo ₄ AlB ₄ + (Sc _{0.75} Mo _{0.25})B ₂ + MoAlB
Zr	Sc	W	-8.165691	-8.169570	-8.168704	N/A	N/A	-8.452316	287	283	284	N/A	N/A	(Zr _{0.75} Sc _{0.25})B ₂ + ScW ₂ B ₄ + WB + WAlB
Zr	Sc	Mn	-7.532131	-7.531966	-7.532358	N/A	N/A	-7.820025	288	288	288	N/A	N/A	(Zr _{0.5} Sc _{0.5})B ₂ + (Zr _{0.75} Sc _{0.25})B ₂ + Mn ₂ AlB ₂
Zr	Sc	Fe	-7.310077	-7.313008	-7.313143	N/A	N/A	-7.662599	353	350	349	N/A	N/A	(Zr _{0.75} Sc _{0.25})B ₂ + (Zr _{0.5} Sc _{0.5})B ₂ + Fe ₂ AlB ₂
Hf	Sc	Sc	-7.499507	-7.499502	-7.499332	-7.555881	-7.573207	-7.599804	100	100	100	44	27	(Hf _{0.5} Sc _{0.5})B ₂ + (Sc _{0.75} Hf _{0.25})B ₂ + AlSc
Hf	Sc	Y	-7.376989	-7.376873	-7.376732	-7.428047	-7.450630	-7.532755	156	156	156	105	82	(Hf _{0.5} Sc _{0.5})B ₂ + AlY ₂ + YB ₂ + Al ₂ Y + (Hf _{0.75} Sc _{0.25})B ₂
Hf	Sc	Ti	-7.895918	-7.895693	-7.896134	-7.939265	-7.944596	-7.957214	61	62	61	18	13	(Ti _{0.83} Sc _{0.17}) ₄ AlB ₆ + (Hf _{0.83} Sc _{0.17}) ₄ AlB ₆
Hf	Sc	Zr	-7.997563	-7.997532	-7.997784	-8.035342	-8.050926	-8.063374	66	66	66	28	12	Al ₃ Zr ₂ + AlSc + (Hf _{0.5} Zr _{0.5})B ₂ + Al ₃ Zr ₄ + (Zr _{0.75} Hf _{0.25})B ₂
Hf	Sc	Hf	-8.271639	-8.271662	-8.271948	N/A	-8.321585	-8.304382	33	33	32	N/A	-17	(Hf _{0.78} Sc _{0.22}) ₃ AlB ₄ + HfB ₂
Hf	Sc	V	-7.944611	-7.946130	-7.946857	-8.008617	-8.024236	-8.096037	151	150	149	87	72	V ₅ B ₆ + V ₃ B ₄ + Al ₃ V + Al ₃ Sc + (Hf _{0.75} Sc _{0.25})B ₂
Hf	Sc	Nb	-8.155450	-8.154813	-8.155531	-8.236927	-8.269797	-8.282901	127	128	127	46	13	NbB + Al ₃ Nb + (Hf _{0.75} Nb _{0.25})B ₂ + (Nb _{0.5} Sc _{0.5})B ₂ + (Hf _{0.75} Sc _{0.25})B ₂
Hf	Sc	Ta	-8.460209	-8.459726	-8.460241	-8.544765	-8.582669	-8.599448	139	140	139	55	17	(Hf _{0.75} Ta _{0.25})B ₂ + Al ₃ Ta + (Ta _{0.5} Sc _{0.5})B ₂ + TaB + (Hf _{0.75} Sc _{0.25})B ₂
Hf	Sc	Cr	-7.825701	-7.829507	-7.829570	N/A	N/A	-8.093210	268	264	264	N/A	N/A	(Hf _{0.5} Sc _{0.5})B ₂ + Cr ₂ AlB ₂ + (Hf _{0.75} Sc _{0.25})B ₂
Hf	Sc	Mo	-8.061396	-8.062436	-8.061688	N/A	N/A	-8.314752	253	252	253	N/A	N/A	Al ₃ Mo ₃ + (Sc _{0.75} Mo _{0.25})B ₂ + Mo ₄ AlB ₄ + MoAlB + (Hf _{0.75} Sc _{0.25})B ₂
Hf	Sc	W	-8.348594	-8.349407	-8.348535	N/A	N/A	-8.637952	289	289	289	N/A	N/A	ScW ₂ B ₄ + WB + WAlB + (Hf _{0.75} Sc _{0.25})B ₂
Hf	Sc	Mn	-7.718186	-7.717318	-7.717696	N/A	N/A	-8.006166	288	289	288	N/A	N/A	(Hf _{0.5} Sc _{0.5})B ₂ + Mn ₂ AlB ₂ + (Hf _{0.75} Sc _{0.25})B ₂
Hf	Sc	Fe	-7.498045	-7.498527	-7.498723	N/A	N/A	-7.848740	351	350	350	N/A	N/A	(Hf _{0.5} Sc _{0.5})B ₂ + Fe ₂ AlB ₂ + (Hf _{0.75} Sc _{0.25})B ₂
V	Sc	Sc	-7.381359	-7.380810	-7.380827	-7.380557	-7.393280	-7.416658	35	36	36	36	23	Al ₂ Sc + VB + ScB ₂ + (Sc _{0.75} V _{0.25})B ₂
V	Sc	Y	-7.226948	-7.226507	-7.227076	-7.190082	-7.240349	-7.336064	109	110	109	146	96	(Y _{0.75} Sc _{0.25})B ₂ + VYB ₄ + Al ₂ Y + VB + (Sc _{0.75} V _{0.25})B ₂
V	Sc	Ti	-7.795279	-7.794913	-7.794721	-7.793093	-7.783920	-7.826240	31	31	32	33	42	(Ti _{0.75} Sc _{0.25})B ₂ + Al ₃ Sc + VB + TiB ₂
V	Sc	Zr	-7.862279	-7.861536	-7.861612	-7.810017	-7.832383	-7.919979	58	58	58	110	88	(Zr _{0.75} Sc _{0.25})B ₂ + Al ₃ Zr + Al ₃ Sc + VB
V	Sc	Hf	-8.141558	-8.140935	-8.140960	-8.094926	-8.113399	-8.190411	49	49	49	95	77	VB + Al ₃ Sc + HfB ₂ + (Hf _{0.75} Sc _{0.25})B ₂
V	Sc	V	-7.857887	-7.857476	-7.857366	N/A	-7.878388	-7.881047	23	24	24	N/A	3	V ₂ B ₃ + (V _{0.75} Sc _{0.25})B ₂ + V ₃ B ₄ + Al ₃ Sc
V	Sc	Nb	-8.039719	-8.039048	-8.039271	-8.042422	-8.063490	-8.100914	61	62	62	58	37	V ₅ B ₆ + (Nb _{0.83} Sc _{0.17}) ₄ AlB ₆ + (Nb _{0.75} Sc _{0.25})B ₂ + Al ₃ Nb + (Nb _{0.5} Sc _{0.5})B ₂
V	Sc	Ta	-8.347686	-8.346814	-8.347281	-8.357544	-8.379474	-8.409684	62	63	62	52	30	(Ta _{0.5} V _{0.5}) ₂ B ₃ + (Ta _{0.5} V _{0.5}) ₃ B ₄ + (V _{0.75} Ta _{0.25}) ₂ B ₃ + Al ₃ Ta + (Ta _{0.5} Sc _{0.5})B ₂
V	Sc	Cr	-7.757108	-7.757854	-7.758296	N/A	N/A	-7.883936	127	126	126	N/A	N/A	Cr ₂ VAlB ₄ + Cr ₂ AlB ₂ + (V _{0.5} Sc _{0.5})B ₂
V	Sc	Mo	-7.969624	-7.971920	-7.972299	N/A	N/A	-8.107079	137	135	135	N/A	N/A	(V _{0.75} Sc _{0.25})B ₂ + MoAlB + (Mo _{0.5} Sc _{0.5})B ₂ + (Mo _{0.5} V _{0.5})B + (Sc _{0.75} Mo _{0.25})B ₂
V	Sc	W	-8.256661	-8.260327	-8.260713	N/A	N/A	-8.431596	175	171	171	N/A	N/A	(V _{0.75} Sc _{0.25})B ₂ + Al ₃ W + (Sc _{0.75} W _{0.25})B ₂ + (W _{0.75} V _{0.25})B ₂ + (W _{0.75} V _{0.25})B ₂
V	Sc	Mn	-7.631122	-7.631808	-7.631715	N/A	N/A	-7.791230	160	159	160	N/A	N/A	(V _{0.75} Sc _{0.25})B ₂ + (V _{0.5} Sc _{0.5})B ₂ + Mn ₂ AlB ₂
V	Sc	Fe	-7.413397	-7.414165	-7.414039	N/A	N/A	-7.633803	220	220	220	N/A	N/A	(V _{0.75} Sc _{0.25})B ₂ + (V _{0.5} Sc _{0.5})B ₂ + Fe ₂ AlB ₂
Nb	Sc	Sc	-7.519602	-7.519239	-7.519132	-7.557312	-7.573882	-7.574437	55	55	55	17	1	(Nb _{0.5} Sc _{0.5}) ₄ AlB ₆ + AlSc + (Sc _{0.75} Nb _{0.25})B ₂
Nb	Sc	Y	-7.382677	-7.382382	-7.382536	-7.383251	-7.434791	-7.490184	108	108	108	107	55	(Y _{0.75} Nb _{0.25})B ₂ + (Nb _{0.5} Y _{0.5})B ₂ + AlY ₂ + Al ₂ Y + (Nb _{0.5} Sc _{0.5})B ₂
Nb	Sc	Ti	-7.907665	-7.906037	-7.906358	-7.924269	-7.932619	-7.936714	29	31	30	12	4	(Nb _{0.75} Ti _{0.25})B + (Nb _{0.5} Sc _{0.5}) ₄ AlB ₆ + Al ₃ Nb + Al ₂ Sc + TiB ₂
Nb	Sc	Zr	-7.997319	-7.995061	-7.995439	-7.991114	-8.017780	-8.027519	30	32	32	36	10	NbB + (Zr _{0.75} Sc _{0.25})B ₂ + Al ₂ Sc + Al ₃ Nb + Al ₂ Zr
Nb	Sc	Hf	-8.272515	-8.270236	-8.270595	-8.266341	-8.292328	-8.303678	31	33	33	37	11	NbB + Al ₃ Nb + (Nb _{0.75} Hf _{0.25})B ₂ + Al ₂ Sc + (Hf _{0.75} Sc _{0.25})B ₂

Nb	Sc	V	-7.945431	-7.946196	-7.945665	-7.984165	-7.996311	-8.044171	99	98	99	60	48	(Nb _{0.75} Sc _{0.25})B ₂ + Al ₃ Nb + V ₃ B ₄ + (Nb _{0.5} Sc _{0.5})B ₂
Nb	Sc	Nb	-8.140641	-8.141379	-8.141297	N/A	-8.214029	-8.206409	66	65	65	N/A	-8	Nb ₃ B ₄ + (Nb _{0.75} Sc _{0.25})B ₂ + Al ₃ Nb + (Nb _{0.5} Sc _{0.5})B ₂
Nb	Sc	Ta	-8.444915	-8.445480	-8.445311	-8.483611	-8.523297	-8.545037	100	100	100	61	22	(Ta _{0.5} Nb _{0.5}) ₃ B ₄ + (Ta _{0.75} Nb _{0.25}) ₃ B ₄ + (Nb _{0.5} Sc _{0.5}) ₂ B ₃ + (Ta _{0.5} Sc _{0.5})B ₂ + Al ₃ Nb
Nb	Sc	Cr	-7.831673	-7.832329	-7.834728	N/A	N/A	-8.028324	197	196	194	N/A	N/A	(Nb _{0.75} Sc _{0.25})B ₂ + Cr ₂ AlB ₂ + (Nb _{0.5} Sc _{0.5})B ₂
Nb	Sc	Mo	-8.053888	-8.055137	-8.055750	N/A	N/A	-8.247891	194	193	192	N/A	N/A	Mo ₄ AlB ₄ + (Nb _{0.75} Sc _{0.25})B ₂ + MoAlB + (Nb _{0.5} Sc _{0.5})B ₂
Nb	Sc	W	-8.337383	-8.338977	-8.340996	N/A	N/A	-8.569917	233	231	229	N/A	N/A	(W _{0.75} Nb _{0.25})B ₂ + (Nb _{0.75} Sc _{0.25})B ₂ + (W _{0.75} Nb _{0.25})B + WAlB + (Nb _{0.5} Sc _{0.5})B ₂
Nb	Sc	Mn	-7.717931	-7.719167	-7.718933	N/A	N/A	-7.941280	223	222	222	N/A	N/A	(Nb _{0.75} Sc _{0.25})B ₂ + Mn ₂ AlB ₂ + (Nb _{0.5} Sc _{0.5})B ₂
Nb	Sc	Fe	-7.501345	-7.501091	-7.500686	N/A	N/A	-7.783854	283	283	283	N/A	N/A	(Nb _{0.75} Sc _{0.25})B ₂ + Fe ₂ AlB ₂ + (Nb _{0.5} Sc _{0.5})B ₂
Ta	Sc	Sc	-7.730332	-7.729885	-7.729958	-7.771591	-7.787821	-7.789554	59	60	60	18	2	(Ta _{0.5} Sc _{0.5}) ₄ AlB ₆ + AlSc + (Sc _{0.75} Ta _{0.25})B ₂
Ta	Sc	Y	-7.592026	-7.591798	-7.592061	-7.590828	-7.642581	-7.701912	110	110	110	111	59	AlY ₂ + (Y _{0.75} Ta _{0.25})B ₂ + TaB + Al ₂ Y + (Ta _{0.5} Sc _{0.5})B ₂
Ta	Sc	Ti	-8.117997	-8.116986	-8.117127	-8.138629	-8.148228	-8.157894	40	41	41	19	10	(Ti _{0.75} Ta _{0.25})B ₂ + (Ta _{0.5} Sc _{0.5})B ₂ + (Ti _{0.75} Sc _{0.25})B ₂ + Al ₃ Sc + (Ta _{0.75} Ti _{0.25})B
Ta	Sc	Zr	-8.205568	-8.204011	-8.204385	-8.198991	-8.227895	-8.247931	42	44	44	49	20	(Zr _{0.75} Sc _{0.25})B ₂ + Al ₃ Zr + Al ₃ Sc + TaB
Ta	Sc	Hf	-8.480100	-8.478521	-8.478980	-8.473366	-8.501676	-8.518363	38	40	39	45	17	Al ₃ Sc + TaB + HfB ₂ + (Hf _{0.75} Sc _{0.25})B ₂
Ta	Sc	V	-8.155534	-8.156152	-8.155266	-8.197243	-8.208820	-8.244746	89	89	89	48	36	(V _{0.75} Ta _{0.25}) ₃ B ₄ + V ₂ B ₃ + Al + Al ₃ Ta + (Ta _{0.5} Sc _{0.5})B ₂
Ta	Sc	Nb	-8.346923	-8.347279	-8.346870	-8.381830	-8.420195	-8.441263	94	94	94	59	21	(Ta _{0.5} Nb _{0.5}) ₃ B ₄ + (Nb _{0.75} Sc _{0.25})B ₂ + (Ta _{0.5} Sc _{0.5})B ₂ + Al ₃ Nb + (Nb _{0.5} Sc _{0.5})B ₂
Ta	Sc	Ta	-8.649349	-8.649256	-8.649082	N/A	-8.726166	-8.726179	77	77	77	N/A	0	(Ta _{0.5} Sc _{0.5})B ₂ + Ta ₃ B ₄ + Al ₃ Ta + (Ta _{0.75} Sc _{0.25})B ₂
Ta	Sc	Cr	-8.036548	-8.042059	-8.044127	N/A	N/A	-8.235548	199	193	191	N/A	N/A	Cr ₄ AlB ₂ + (Ta _{0.5} Sc _{0.5})B ₂ + (Ta _{0.75} Sc _{0.25})B ₂
Ta	Sc	Mo	-8.259296	-8.260974	-8.261608	N/A	N/A	-8.459857	201	199	198	N/A	N/A	(Mo _{0.75} Ta _{0.25})B + (Mo _{0.75} Ta _{0.25})B ₂ + MoAlB + (Ta _{0.5} Sc _{0.5})B ₂ + (Ta _{0.75} Sc _{0.25})B ₂
Ta	Sc	W	-8.540368	-8.543522	-8.544444	N/A	N/A	-8.781773	241	238	237	N/A	N/A	(Ta _{0.5} W _{0.5})B ₂ + (Ta _{0.75} Sc _{0.25})B ₂ + (W _{0.75} Ta _{0.25})B + WAlB + (Ta _{0.5} Sc _{0.5})B ₂
Ta	Sc	Mn	-7.927829	-7.929000	-7.928731	N/A	N/A	-8.148504	221	220	220	N/A	N/A	(Ta _{0.75} Sc _{0.25})B ₂ + (Ta _{0.5} Sc _{0.5})B ₂ + Mn ₂ AlB ₂
Ta	Sc	Fe	-7.711227	-7.711295	-7.711208	N/A	N/A	-7.991078	280	280	280	N/A	N/A	(Ta _{0.5} Sc _{0.5})B ₂ + Fe ₂ AlB ₂ + (Ta _{0.75} Sc _{0.25})B ₂
Cr	Sc	Sc	-7.392457	-7.392169	-7.392294	-7.337415	-7.358312	-7.410319	18	18	18	73	52	Cr _{4/3} Sc _{2/3} AlB ₂ + ScB ₂
Cr	Sc	Y	-7.234274	-7.233170	-7.234391	-7.137061	-7.213248	-7.358524	124	125	124	221	145	AlY ₂ + CrYB ₄ + Al ₂ Y + CrB + ScB ₂
Cr	Sc	Ti	-7.803334	-7.802285	-7.802134	-7.742160	-7.732811	-7.818092	15	16	16	76	85	(Ti _{0.75} Sc _{0.25})B ₂ + Al ₃ Sc + CrB + TiB ₂
Cr	Sc	Zr	-7.864474	-7.863062	-7.863151	-7.750044	-7.776917	-7.911831	47	49	49	162	135	(Zr _{0.75} Sc _{0.25})B ₂ + Al ₃ Zr + CrB + Al ₃ Sc
Cr	Sc	Hf	-8.144321	-8.142319	-8.142707	-8.035415	-8.056741	-8.184311	40	42	42	149	128	Cr ₄ AlB ₄ + Al ₃ Sc + AlCr ₂ + HfB ₂ + (Hf _{0.75} Sc _{0.25})B ₂
Cr	Sc	V	-7.873449	-7.873739	-7.874122	-7.855447	-7.829124	-7.888682	15	15	15	33	60	(V _{0.5} Cr _{0.5})B + Cr ₂ V ₂ AlB ₆ + (V _{0.75} Cr _{0.25})B + Al ₄₅ Cr ₇ + (V _{0.5} Sc _{0.5})B ₂
Cr	Sc	Nb	-8.048721	-8.049049	-8.049525	-7.990732	-8.006985	-8.093576	45	45	44	103	87	Cr ₄ AlB ₄ + (Nb _{0.83} Sc _{0.17}) ₄ AlB ₆ + (Nb _{0.75} Sc _{0.25})B ₂ + Al ₃ Nb + (Nb _{0.5} Sc _{0.5})B ₂
Cr	Sc	Ta	-8.357024	-8.357264	-8.357617	-8.306610	-8.322590	-8.399092	42	42	41	92	77	Cr ₂ AlB ₂ + Ta ₃ B ₄ + Al ₃ Ta + (Ta _{0.5} Sc _{0.5})B ₂ + (Ta _{0.75} Sc _{0.25})B ₂
Cr	Sc	Cr	-7.777822	-7.779603	-7.779108	N/A	N/A	-7.816986	39	37	38	N/A	N/A	Cr ₂ AlB ₂ + CrSc ₂ B ₆ + CrB ₄ + Cr ₄ AlB ₄
Cr	Sc	Mo	-7.984234	-7.990532	-7.989549	N/A	N/A	-8.071032	87	80	81	N/A	N/A	Cr ₄ AlB ₄ + (Cr _{0.75} Mo _{0.25})B + (Mo _{0.75} Cr _{0.25})B ₂ + (Mo _{0.5} Sc _{0.5})B ₂ + MoAlB
Cr	Sc	W	-8.271043	-8.279373	-8.278138	N/A	N/A	-8.396855	126	117	119	N/A	N/A	(Sc _{0.75} W _{0.25})B ₂ + (Cr _{0.5} W _{0.5})AlB + Cr ₂ AlB ₂ + (Cr _{0.5} W _{0.5})B ₂ + (W _{0.75} Cr _{0.25})B ₂
Cr	Sc	Mn	-7.647336	-7.648995	-7.648198	N/A	N/A	-7.748265	101	99	100	N/A	N/A	CrMn ₂ B ₄ + (Cr _{0.75} Mn _{0.25})B ₂ + CrSc ₂ B ₆ + (Mn _{0.75} Cr _{0.25})B ₄ + (Mn _{0.67} Cr _{0.33}) ₂ AlB ₂
Cr	Sc	Fe	-7.420890	-7.422296	-7.425628	N/A	N/A	-7.577929	157	156	152	N/A	N/A	CrFe ₂ B ₄ + (Fe _{0.67} Cr _{0.33}) ₂ AlB ₂ + CrSc ₂ B ₆ + (Cr _{0.75} Fe _{0.25})B ₄ + FeB
Mo	Sc	Sc	-7.572883	-7.573386	-7.573199	-7.563673	-7.588624	-7.589585	17	16	16	26	1	AlSc + Al ₂ Sc + (Sc _{0.75} Mo _{0.25})B ₂ + AlMo ₃
Mo	Sc	Y	-7.426258	-7.426359	-7.426460	-7.383141	-7.438846	-7.495089	69	69	69	112	56	MoYB ₄ + AlY ₂ + Al ₂ Y + Mo _{4/3} Y _{2/3} AlB ₂ + (Sc _{0.75} Mo _{0.25})B ₂
Mo	Sc	Ti	-7.956381	-7.955554	-7.955022	-7.919579	-7.931715	-7.979026	23	23	24	59	47	(Mo _{0.75} Ti _{0.25})B + (Ti _{0.75} Sc _{0.25})B ₂ + Al ₈ Mo ₃ + (Sc _{0.75} Mo _{0.25})B ₂ + AlMo ₃
Mo	Sc	Zr	-8.033026	-8.010815	-8.031462	-7.957551	-7.995375	-8.068598	36	58	37	111	73	Al ₈ Mo ₃ + (Zr _{0.75} Sc _{0.25})B ₂ + AlMo ₃ + MoB
Mo	Sc	Hf	-8.310207	-8.309140	-8.308396	-8.235703	-8.271543	-8.347052	37	38	39	111	76	Al ₈ Mo ₃ + AlMo ₃ + MoB + (Hf _{0.75} Sc _{0.25})B ₂
Mo	Sc	V	-8.007383	-8.008919	-8.009615	-7.996542	-7.996953	-8.044793	37	36	35	48	48	(V _{0.75} Sc _{0.25})B ₂ + MoAlB + (V _{0.5} Mo _{0.5})B + Al ₂₂ Mo ₅ + (Sc _{0.75} Mo _{0.25})B ₂
Mo	Sc	Nb	-8.191803	-8.193530	-8.194202	-8.159250	-8.189692	-8.246573	55	53	52	87	57	Al ₈ Mo ₃ + (Nb _{0.75} Sc _{0.25})B ₂ + (Mo _{0.75} Nb _{0.25})B ₂ + MoAlB + (Nb _{0.5} Sc _{0.5})B ₂
Mo	Sc	Ta	-8.496978	-8.498704	-8.499224	-8.465324	-8.497455	-8.563075	66	64	64	98	66	MoAlB + (Mo _{0.5} Ta _{0.5})B + Al ₂₂ Mo ₅ + (Ta _{0.5} Sc _{0.5})B ₂ + (Ta _{0.75} Sc _{0.25})B ₂
Mo	Sc	Cr	-7.897294	-7.898069	-7.897459	N/A	N/A	-7.994666	97	97	97	N/A	N/A	(Cr _{0.5} Mo _{0.5})AlB + Cr ₄ AlB ₄ + (Cr _{0.75} Mo _{0.25})B ₂ + (Mo _{0.5} Sc _{0.5})B ₂ + MoAlB
Mo	Sc	Mo	-8.108869	-8.114497	-8.113378	N/A	N/A	-8.208362	99	94	95	N/A	N/A	(Mo _{0.5} Sc _{0.5})B ₂ + Mo ₄ AlB ₄ + MoB ₂ + MoAlB

Mo	Sc	W	-8.391750	-8.398511	-8.397223	N/A	N/A	-8.565244	173	167	168	N/A	N/A	(Mo _{0.5} W _{0.5})B ₂ + (Mo _{0.5} W _{0.5})AlB + (W _{0.75} Mo _{0.25})B ₂ + (Sc _{0.75} W _{0.25})B ₂ + (Mo _{0.5} W _{0.5})B
Mo	Sc	Mn	-7.777586	-7.778714	-7.778775	N/A	N/A	-7.901750	124	123	123	N/A	N/A	(Mo _{0.5} Sc _{0.5})B ₂ + MoB ₂ + Mn ₂ AlB ₂
Mo	Sc	Fe	-7.552469	-7.554054	-7.553810	N/A	N/A	-7.744324	192	190	191	N/A	N/A	(Mo _{0.5} Sc _{0.5})B ₂ + Fe ₂ AlB ₂ + MoB ₂
W	Sc	Sc	-7.797503	-7.798093	-7.797946	-7.787760	-7.814325	-7.821531	24	23	24	34	7	(Sc _{0.75} W _{0.25})B ₂ + Al ₃ Sc + Al ₂ Sc + W
W	Sc	Y	-7.649513	-7.649836	-7.650012	-7.606215	-7.659712	-7.730669	81	81	81	124	71	W _{4/3} Y _{2/3} AlB ₂ + ScW ₂ B ₄ + (Sc _{0.75} W _{0.25})B ₂ + WY ₃ B ₇ + Al ₂ Y
W	Sc	Ti	-8.175792	-8.174661	-8.174303	-8.135276	-8.151388	-8.196517	21	22	22	61	45	(W _{0.75} Ti _{0.25})B + (Ti _{0.75} Sc _{0.25})B ₂ + Al ₃ Sc + Al ₃ W + (Sc _{0.75} W _{0.25})B ₂
W	Sc	Zr	-8.250180	-8.249278	-8.248666	-8.168744	-8.210925	-8.280972	31	32	32	112	70	Al ₅ W + (Zr _{0.75} Sc _{0.25})B ₂ + W ₂ B + WB
W	Sc	Hf	-8.526355	-8.525179	-8.524554	-8.444711	-8.484921	-8.559426	33	34	35	115	75	W ₂ B + Al ₅ W + WB + (Hf _{0.75} Sc _{0.25})B ₂
W	Sc	V	-8.221999	-8.222997	-8.223955	-8.206591	-8.209920	-8.263664	42	41	40	57	54	(V _{0.75} Sc _{0.25})B ₂ + Al ₅ W + (Sc _{0.75} W _{0.25})B ₂ + (W _{0.5} V _{0.5})B + (W _{0.75} V _{0.25})B
W	Sc	Nb	-8.400847	-8.403392	-8.403887	-8.362028	-8.396530	-8.463412	63	60	60	101	67	Al ₅ W + (Nb _{0.75} Sc _{0.25})B ₂ + (W _{0.75} Nb _{0.25})B + Al ₃ Nb + (Nb _{0.5} Sc _{0.5})B ₂
W	Sc	Ta	-8.703525	-8.706006	-8.706387	-8.662885	-8.699031	-8.775984	72	70	70	113	77	Al ₅ W + (Ta _{0.75} Sc _{0.25})B ₂ + (W _{0.75} Ta _{0.25})B + (W _{0.5} Ta _{0.5})B + (Ta _{0.5} Sc _{0.5})B ₂
W	Sc	Cr	-8.108786	-8.109985	-8.109743	N/A	N/A	-8.212548	104	103	103	N/A	N/A	(Sc _{0.75} W _{0.25})B ₂ + (Cr _{0.5} W _{0.5})AlB + Cr ₂ AlB ₂ + (W _{0.5} Cr _{0.5})B + (W _{0.75} Cr _{0.25})B ₂
W	Sc	Mo	-8.314618	-8.320070	-8.318891	N/A	N/A	-8.455004	140	135	136	N/A	N/A	(Mo _{0.5} W _{0.5})B ₂ + (Mo _{0.5} Sc _{0.5})B ₂ + (Mo _{0.5} W _{0.5})AlB + (Mo _{0.5} W _{0.5})B
W	Sc	W	-8.593764	-8.600278	-8.599201	N/A	N/A	-8.744329	151	144	145	N/A	N/A	ScW ₂ B ₄ + (Sc _{0.75} W _{0.25})B ₂ + WB ₂ + WAlB
W	Sc	Mn	-7.992526	-7.993597	-7.993858	N/A	N/A	-8.117781	125	124	124	N/A	N/A	(Sc _{0.75} W _{0.25})B ₂ + WB ₂ + Mn ₂ AlB ₂
W	Sc	Fe	-7.765105	-7.768538	-7.767285	N/A	N/A	-7.960355	195	192	193	N/A	N/A	WB ₂ + Fe ₂ AlB ₂ + (Sc _{0.75} W _{0.25})B ₂
Mn	Sc	Sc	-7.350150	-7.350241	-7.350488	-7.254475	-7.274742	-7.374926	25	25	24	120	100	Mn _{4/3} Sc _{2/3} AlB ₂ + ScB ₂
Mn	Sc	Y	-7.188657	-7.187465	-7.188512	-7.070244	-7.149613	-7.289129	100	102	101	219	140	Mn _{4/3} Y _{2/3} AlB ₂ + MnYB ₄ + MnY ₃ B ₇ + Al ₂ Y + ScB ₂
Mn	Sc	Ti	-7.761595	-7.759651	-7.760022	-7.656179	-7.642428	-7.777223	16	18	17	121	135	Mn _{4/3} Sc _{2/3} AlB ₂ + TiB ₂
Mn	Sc	Zr	-7.818897	-7.816964	-7.817397	-7.669381	-7.697537	-7.871787	53	55	54	202	174	Mn _{4/3} Zr _{2/3} AlB ₂ + Mn _{4/3} Sc _{2/3} AlB ₂ + (Zr _{0.75} Sc _{0.25})B ₂
Mn	Sc	Hf	-8.099504	-8.097505	-8.097898	-7.952053	-7.974028	-8.141995	42	44	44	190	168	Mn _{4/3} Hf _{2/3} AlB ₂ + Mn _{4/3} Sc _{2/3} AlB ₂ + (Hf _{0.75} Sc _{0.25})B ₂
Mn	Sc	V	-7.835076	-7.838152	-7.837360	-7.773725	-7.744512	-7.829973	-5	-8	-7	56	85	(Mn _{0.67} V _{0.33}) ₂ AlB ₂ + Mn _{4/3} Sc _{2/3} VAlB ₄ + (V _{0.75} Sc _{0.25})B ₂
Mn	Sc	Nb	-8.002636	-8.006781	-8.005956	-7.910978	-7.926213	-8.032196	30	25	26	121	106	(Nb _{0.83} Sc _{0.17}) ₄ AlB ₆ + (Nb _{0.75} Sc _{0.25})B ₂ + Mn ₂ AlB ₂ + (Nb _{0.5} Sc _{0.5})B ₂
Mn	Sc	Ta	-8.310296	-8.314408	-8.313673	-8.225803	-8.241111	-8.344562	34	30	31	119	103	Ta ₃ B ₄ + Al ₁₁ Mn ₄ + (Ta _{0.75} Sc _{0.25})B ₂ + (Ta _{0.5} Sc _{0.5})B ₂ + Mn ₂ AlB ₂
Mn	Sc	Cr	-7.735013	-7.738567	-7.738579	N/A	N/A	-7.785256	50	47	47	N/A	N/A	(Cr _{0.75} Mn _{0.25})B ₂ + CrSc ₂ B ₆ + (Cr _{0.67} Mn _{0.33}) ₂ AlB ₂ + (Mn _{0.67} Cr _{0.33}) ₂ AlB ₂
Mn	Sc	Mo	-7.938550	-7.941125	-7.941387	N/A	N/A	-8.004798	66	64	63	N/A	N/A	(Mo _{0.5} Sc _{0.5})B ₂ + (Mn _{0.67} Mo _{0.33}) ₂ AlB ₂ + MoB ₂
Mn	Sc	W	-8.226319	-8.229667	-8.230077	N/A	N/A	-8.327139	101	97	97	N/A	N/A	(Sc _{0.75} W _{0.25})B ₂ + WB ₂ + (W _{0.75} Mn _{0.25})B + WAlB + Mn ₂ AlB ₂
Mn	Sc	Mn	-7.605835	-7.610484	-7.607357	N/A	N/A	-7.648654	43	38	41	N/A	N/A	MnB ₄ + Mn ₄ AlB ₄ + (Sc _{0.75} Mn _{0.25})B ₂ + Mn ₂ AlB ₂
Mn	Sc	Fe	-7.380371	-7.377787	-7.377804	N/A	N/A	-7.506470	126	129	129	N/A	N/A	(Mn _{0.67} Fe _{0.33}) ₂ AlB ₂ + (Fe _{0.67} Mn _{0.33}) ₂ AlB ₂ + (Sc _{0.75} Mn _{0.25})B ₂ + MnB ₄ + FeB
Fe	Sc	Sc	-7.254235	-7.254246	-7.254296	-7.116718	-7.144841	-7.270740	17	16	16	154	126	Fe _{4/3} Sc _{2/3} AlB ₂ + ScB ₂
Fe	Sc	Y	-7.093553	-7.093529	-7.093548	-6.956191	-7.029529	-7.188030	94	95	94	232	159	FeYB ₄ + FeY ₃ B ₇ + Fe ₂ YB ₂ + Al ₂ Y + ScB ₂
Fe	Sc	Ti	-7.654632	-7.447912	-7.653448	-7.514636	-7.502540	-7.677636	23	230	24	163	175	(Ti _{0.75} Sc _{0.25})B ₂ + Fe ₂ AlB ₂ + AlFe
Fe	Sc	Zr	-7.706554	-7.706081	-7.706233	-7.526654	-7.563587	-7.773124	67	67	67	246	210	(Zr _{0.75} Sc _{0.25})B ₂ + AlFe + Fe ₂ AlB ₂
Fe	Sc	Hf	-7.987936	-7.987397	-7.987484	-7.808814	-7.835100	-8.051577	64	64	64	243	216	AlFe + Fe ₂ AlB ₂ + (Hf _{0.75} Sc _{0.25})B ₂
Fe	Sc	V	-7.729959	-7.729084	-7.733091	-7.638676	-7.604097	-7.727093	-3	1	-3	88	123	V ₂ B ₃ + Fe ₂ VAlB ₄ + Fe _{4/3} Sc _{2/3} VAlB ₄ + (V _{0.75} Sc _{0.25})B ₂ + Al ₃ Fe ₄ Sc
Fe	Sc	Nb	-7.896193	-7.900146	-7.899599	-7.769378	-7.783138	-7.937326	41	37	38	168	154	(Nb _{0.75} Sc _{0.25})B ₂ + Fe ₂ AlB ₂ + AlFe
Fe	Sc	Ta	-8.204978	-8.209034	-8.208435	-8.085034	-8.098868	-8.244383	39	35	36	159	146	Fe ₂ AlB ₂ + (Ta _{0.75} Sc _{0.25})B ₂ + AlFe
Fe	Sc	Cr	-7.614890	-7.615745	-7.615916	N/A	N/A	-7.667060	52	51	51	N/A	N/A	(Fe _{0.67} Cr _{0.33}) ₂ AlB ₂ + CrSc ₂ B ₆ + CrB ₄ + CrB
Fe	Sc	Mo	-7.822403	-7.818742	-7.819646	N/A	N/A	-7.899003	77	80	79	N/A	N/A	(Mo _{0.5} Sc _{0.5})B ₂ + Mo ₄ AlB ₄ + Fe ₂ AlB ₂ + MoB ₂ + MoAlB
Fe	Sc	W	-8.114063	-8.108596	-8.110535	N/A	N/A	-8.221729	108	113	111	N/A	N/A	WB ₂ + Fe ₂ AlB ₂ + (Sc _{0.75} W _{0.25})B ₂ + FeW ₂ B ₂ + WAlB
Fe	Sc	Mn	-7.493631	-7.493676	-7.493594	N/A	N/A	-7.558666	65	65	65	N/A	N/A	(Mn _{0.67} Fe _{0.33}) ₂ AlB ₂ + (Sc _{0.75} Mn _{0.25})B ₂ + MnB ₄ + FeB + Mn ₄ AlB ₄
Fe	Sc	Fe	-7.258485	-7.252892	-7.256910	N/A	N/A	-7.365248	107	112	108	N/A	N/A	Fe ₂ B ₇ + Fe ₂ AlB ₂ + FeB + ScB ₂

Table S5. Calculated energy (E) and stability at 2000 K (ΔG_{cp}^{s-MAB} , $\Delta G_{cp}^{partial\ disorder}$, $\Delta G_{cp}^{disorder}$) for M2 = Y in *s*-MAB, *s*-MAB with disorder, and MAB with disorder for 416 MAB phases along with corresponding energy for their competing phases and identified set of most competing phases. Phases modelled with solid solution disorder have a contribution from configurational entropy evaluated at 2000 K. Competing phases in bold highlight when a MAB phase is part of the set of most competing phases.

M1	M2	M3	Energy (eV/atom)					ΔH_{cp} (meV/atom)					Set of most competing phases	
			s-MAB (no. 191)	s-MAB (no. 194)	s-MAB (no. 166)	s-MAB disorder	MAB disorder	Competing phases	s-MAB (no. 191)	s-MAB (no. 194)	s-MAB (no. 166)	s-MAB partial disorder		
Sc	Y	Sc	-7.028687	-7.028790	-7.028606	N/A	-7.034556	-7.059531	31	31	31	N/A	25	AlSc ₂ + AlY ₂ + Al ₂ Y + ScB ₂
Sc	Y	Y	-6.912034	-6.911524	-6.911909	-6.921888	-6.929374	-6.964135	52	53	52	42	35	(Sc _{0.75} Y _{0.25})B ₂ + (Y _{0.75} Sc _{0.25})B ₂ + AlY ₂ + Al ₂ Y
Sc	Y	Ti	-7.417765	-7.417870	-7.418028	-7.442703	-7.389878	-7.482714	65	65	65	40	93	(Ti _{0.5} Sc _{0.5})B ₂ + (Ti _{0.75} Sc _{0.25})B ₂ + AlY ₂ + AlSc ₂ + Al ₂ Y
Sc	Y	Zr	-7.524397	-7.524410	-7.524700	-7.541404	-7.508478	-7.580848	56	56	56	39	72	(Zr _{0.75} Sc _{0.25})B ₂ + (Zr _{0.5} Sc _{0.5})B ₂ + AlSc ₂ + AlY ₂ + Al ₂ Y
Sc	Y	Hf	-7.799003	-7.798996	-7.799285	-7.814458	-7.774862	-7.860059	61	61	61	46	85	(Hf _{0.5} Sc _{0.5})B ₂ + AlSc ₂ + AlY ₂ + Al ₂ Y + (Hf _{0.75} Sc _{0.25})B ₂
Sc	Y	V	-7.482862	-7.483259	-7.482989	-7.543890	-7.491279	-7.584450	102	101	101	41	93	(V _{0.5} Sc _{0.5})B ₂ + VYB ₄ + Al ₂ Y + VB + (Sc _{0.75} V _{0.25})B ₂
Sc	Y	Nb	-7.705820	-7.706239	-7.705869	-7.789723	-7.754926	-7.813046	107	107	107	23	58	AlY ₂ + Al ₂ Y + NbB + (Nb _{0.5} Sc _{0.5})B ₂
Sc	Y	Ta	-8.017738	-8.018116	-8.017688	-8.106733	-8.070714	-8.139557	122	121	122	33	69	AlY ₂ + TaB + Al ₂ Y + (Ta _{0.5} Sc _{0.5})B ₂
Sc	Y	Cr	-7.374243	-7.373667	-7.373906	N/A	N/A	-7.556013	182	182	182	N/A	N/A	CrAlB₄ + Al ₃ Y + CrYB ₄ + Al ₂ Y + ScB ₂
Sc	Y	Mo	-7.622658	-7.622009	-7.622101	N/A	N/A	-7.815443	193	193	193	N/A	N/A	(Mo _{0.5} Sc _{0.5})B ₂ + Mo_{4/3}Y_{2/3}AlB₂ + (Sc _{0.75} Mo _{0.25})B ₂
Sc	Y	W	-7.918710	-7.918083	-7.918320	N/A	N/A	-8.144239	226	226	226	N/A	N/A	WAlB + W_{4/3}Y_{2/3}AlB₂ + ScW ₂ B ₄ + (Sc _{0.75} W _{0.25})B ₂ + YB ₄
Sc	Y	Mn	-7.253955	-7.254114	-7.254248	N/A	N/A	-7.479964	226	226	226	N/A	N/A	MnYB ₄ + ScB ₂ + Mn_{4/3}Sc_{2/3}AlB₂
Sc	Y	Fe	-7.039080	-7.039838	-7.040288	N/A	N/A	-7.322474	283	283	282	N/A	N/A	Fe_{4/3}Sc_{2/3}AlB₂ + FeYB ₄ + ScB ₂
Y	Y	Sc	N/A	N/A	N/A	N/A	-6.966504	-7.004262	N/A	N/A	N/A	N/A	38	(Sc _{0.75} Y _{0.25})B ₂ + (Y _{0.75} Sc _{0.25})B ₂ + AlY ₂ + Al ₂ Y
Y	Y	Ti	N/A	N/A	N/A	N/A	-7.294029	-7.401366	N/A	N/A	N/A	N/A	107	AlY ₂ + YB ₂ + Al ₂ Y + TiB ₂
Y	Y	Zr	N/A	N/A	N/A	N/A	-7.444342	-7.505269	N/A	N/A	N/A	N/A	61	(Zr _{0.5} Y _{0.5})B ₂ + (Zr _{0.75} Y _{0.25})B ₂ + AlY ₂ + Al ₂ Y
Y	Y	Hf	N/A	N/A	N/A	N/A	-7.701746	-7.772758	N/A	N/A	N/A	N/A	71	(Y _{0.75} Hf _{0.25})B ₂ + (Hf _{0.75} Y _{0.25})B ₂ + AlY ₂ + Al ₂ Y
Y	Y	V	N/A	N/A	N/A	N/A	-7.379240	-7.497948	N/A	N/A	N/A	N/A	119	VYB ₄ + AlY ₂ + Al ₂ Y + VB
Y	Y	Nb	N/A	N/A	N/A	N/A	-7.665755	-7.681024	N/A	N/A	N/A	N/A	15	(Nb _{0.5} Y _{0.5})B ₂ + AlY ₂ + Al ₂ Y + NbB
Y	Y	Ta	N/A	N/A	N/A	N/A	-7.975403	-8.000900	N/A	N/A	N/A	N/A	25	(Ta _{0.5} Y _{0.5})B ₂ + (Y _{0.75} Ta _{0.25})B ₂ + Al ₂ Y + TaB
Ti	Y	Sc	-7.277605	-7.277933	-7.277903	-7.311520	-7.264395	-7.345988	68	68	68	34	82	(Ti _{0.5} Sc _{0.5})B ₂ + (Sc _{0.75} Ti _{0.25})B ₂ + AlY ₂ + AlSc ₂ + Al ₂ Y
Ti	Y	Y	-7.145296	-7.145205	-7.145163	-7.132526	-7.136597	-7.225351	80	80	80	93	89	AlY ₂ + YB ₂ + Al ₂ Y + TiB ₂
Ti	Y	Ti	-7.681461	-7.682072	-7.681937	N/A	-7.637243	-7.711727	30	30	30	N/A	74	Ti ₃ B ₄ + AlY ₂ + Al ₂ Y + TiB ₂
Ti	Y	Zr	-7.772564	-7.773127	-7.773036	-7.776980	-7.733360	-7.803801	31	31	31	27	70	(Zr _{0.75} Ti _{0.25})B ₂ + AlY ₂ + Al ₃ Zr ₄ + Al ₂ Y + TiB ₂
Ti	Y	Hf	-8.048925	-8.049553	-8.049407	-8.056464	-8.005243	-8.081565	33	32	32	25	76	(Hf _{0.75} Ti _{0.25})B ₂ + (Ti _{0.5} Hf _{0.5})B ₂ + AlY ₂ + Al ₂ Y + Al ₃ Hf ₄
Ti	Y	V	-7.745556	-7.744438	-7.744573	-7.811032	-7.725860	-7.845700	100	101	101	35	120	(Ti _{0.5} V _{0.5})B ₂ + V ₅ B ₆ + (Ti _{0.75} V _{0.25})B ₂ + VYB ₄ + Al ₂ Y
Ti	Y	Nb	-7.948264	-7.947288	-7.947730	-8.006678	-7.957924	-8.017317	69	70	70	11	59	Nb ₃ B ₄ + (Nb _{0.75} Ti _{0.25}) ₃ B ₄ + (Y _{0.5} Nb _{0.5})B ₂ + (Ti _{0.75} Nb _{0.25})B ₂ + Al ₂ Y
Ti	Y	Ta	-8.255814	-8.254937	-8.255336	-8.321331	-8.273361	-8.343228	87	88	88	22	70	(Ti _{0.5} Ta _{0.5})B ₂ + (Y _{0.5} Ta _{0.5})B ₂ + (Ti _{0.75} Ta _{0.25})B ₂ + Al ₂ Y + TaB
Ti	Y	Cr	-7.635280	-7.636656	-7.636523	N/A	N/A	-7.824211	189	188	188	N/A	N/A	CrYB ₄ + Al ₃ Y + CrAlB₄ + Al ₂ Y + TiB ₂
Ti	Y	Mo	-7.864576	-7.865391	-7.865333	N/A	N/A	-8.043682	179	178	178	N/A	N/A	(Ti _{0.75} Mo _{0.25})B ₂ + Mo₄AlB₄ + Mo_{4/3}Y_{2/3}AlB₂ + MoYB ₄ + MoAlB
Ti	Y	W	-8.153925	-8.154622	-8.154555	N/A	N/A	-8.366313	212	212	212	N/A	N/A	WB + (Ti _{0.75} W _{0.25})B ₂ + W_{4/3}Y_{2/3}AlB₂ + YB ₄ + WAlB
Ti	Y	Mn	-7.518418	-7.516830	-7.516906	N/A	N/A	-7.734948	217	218	218	N/A	N/A	MnYB ₄ + Mn_{4/3}Y_{2/3}AlB₂ + Mn₂AlB₂ + TiB ₂
Ti	Y	Fe	-7.300414	-7.302127	-7.301894	N/A	N/A	-7.578634	278	277	277	N/A	N/A	FeYB ₄ + Fe_{4/3}Y_{2/3}AlB₂ + Fe₂AlB₂ + TiB ₂
Zr	Y	Sc	-7.320731	-7.320884	-7.321080	-7.381198	-7.350120	-7.417449	97	97	96	36	67	(Sc _{0.75} Zr _{0.25})B ₂ + (Sc _{0.5} Zr _{0.5})B ₂ + AlSc ₂ + AlY ₂ + Al ₂ Y

Zr	Y	Y	-7.210270	-7.210314	-7.210456	-7.244538	-7.246036	-7.298812	89	88	88	54	53	(Y _{0.5} Zr _{0.5})B ₂ + (Y _{0.75} Zr _{0.25})B ₂ + AlY ₂ + Al ₂ Y
Zr	Y	Ti	-7.708348	-7.708783	-7.709012	-7.746835	-7.699892	-7.775415	67	67	66	29	76	(Zr _{0.75} Ti _{0.25})B ₂ + AlY ₂ + Al ₃ Zr ₄ + Al ₂ Y + TiB ₂
Zr	Y	Zr	-7.825267	-7.825756	-7.825693	N/A	-7.831396	-7.855058	30	29	29	N/A	24	AlY ₂ + Al ₃ Zr ₄ + Al ₂ Y + ZrB ₂
Zr	Y	Hf	-8.097470	-8.098055	-8.098035	-8.130203	-8.094243	-8.158563	61	61	61	28	64	(Hf _{0.5} Zr _{0.5})B ₂ + (Hf _{0.75} Zr _{0.25})B ₂ + AlY ₂ + Al ₂ Y + Al ₃ Zr ₄
Zr	Y	V	-7.757256	-7.756669	-7.757019	-7.808992	-7.767200	-7.888593	131	132	132	80	121	V ₂ B ₃ + (Zr _{0.75} Y _{0.25})B ₂ + Al ₂ Y + ZrB ₂
Zr	Y	Nb	-7.979774	-7.979364	-7.980010	-8.053679	-8.028721	-8.066420	87	87	86	13	38	(Zr _{0.75} Nb _{0.25})B ₂ + Nb ₃ B ₄ + (Nb _{0.5} Y _{0.5})B ₂ + Al ₂ Y + NbB
Zr	Y	Ta	-8.285412	-8.285483	-8.285782	-8.361575	-8.338357	-8.386400	101	101	101	25	48	(Zr _{0.75} Ta _{0.25})B ₂ + Ta ₃ B ₄ + (Ta _{0.5} Y _{0.5})B ₂ + Al ₂ Y + TaB
Zr	Y	Cr	-7.639764	-7.640701	-7.640500	N/A	N/A	-7.878532	239	238	238	N/A	N/A	CrYB ₄ + Al ₃ Y + Cr₄AlB₄ + Al ₂ Y + ZrB ₂
Zr	Y	Mo	-7.881655	-7.882382	-7.882457	N/A	N/A	-8.094962	213	213	213	N/A	N/A	Mo₄AlB₄ + Mo_{4/3}Y_{2/3}AlB₂ + MoYB ₄ + MoAlB + ZrB ₂
Zr	Y	W	-8.171179	-8.171723	-8.171590	N/A	N/A	-8.416349	245	245	245	N/A	N/A	W_{4/3}Y_{2/3}AlB₂ + YB ₄ + WB + WAlB + ZrB ₂
Zr	Y	Mn	-7.529198	-7.527721	-7.527732	N/A	N/A	-7.789269	260	262	262	N/A	N/A	MnYB ₄ + Mn_{4/3}Y_{2/3}AlB₂ + Mn₂AlB₂ + ZrB ₂
Zr	Y	Fe	-7.312642	-7.313113	-7.313285	N/A	N/A	-7.632954	320	320	320	N/A	N/A	Fe_{4/3}Y_{2/3}AlB₂ + FeYB ₄ + Fe₂AlB₂ + ZrB ₂
Hf	Y	Sc	-7.500684	-7.500943	-7.501346	-7.564003	-7.526492	-7.605339	105	104	104	41	79	(Hf _{0.5} Sc _{0.5})B ₂ + AlSc ₂ + (Sc _{0.75} Hf _{0.25})B ₂ + AlY ₂ + Al ₂ Y
Hf	Y	Y	-7.387629	-7.387803	-7.387848	-7.416171	-7.416285	-7.473617	86	86	86	57	57	(Y _{0.75} Hf _{0.25})B ₂ + (Hf _{0.75} Y _{0.25})B ₂ + AlY ₂ + Al ₂ Y
Hf	Y	Ti	-7.889401	-7.889773	-7.889871	-7.937120	-7.881888	-7.961670	72	72	72	25	80	(Ti _{0.75} Hf _{0.25})B ₂ + (Hf _{0.5} Ti _{0.5})B ₂ + AlY ₂ + Al ₂ Y + Al ₃ Hf ₄
Hf	Y	Zr	-8.002435	-8.002750	-8.002631	-8.040461	-8.005795	-8.069289	67	67	67	29	63	(Hf _{0.5} Zr _{0.5})B ₂ + AlY ₂ + Al ₂ Y + Al ₃ Zr ₄ + (Zr _{0.75} Hf _{0.25})B ₂
Hf	Y	Hf	-8.274471	-8.274811	-8.274803	N/A	-8.270486	-8.303684	29	29	29	N/A	33	AlY ₂ + Al ₃ Hf ₄ + Al ₂ Y + HfB ₂
Hf	Y	V	-7.940445	-7.939935	-7.940208	-8.002986	-7.952119	-8.069512	129	130	129	67	117	V ₂ B ₃ + (Hf _{0.75} Y _{0.25})B ₂ + Al ₂ Y + HfB ₂
Hf	Y	Nb	-8.158778	-8.158256	-8.159020	-8.237237	-8.207543	-8.249715	91	91	91	12	42	(Nb _{0.5} Y _{0.5})B ₂ + Nb ₃ B ₄ + (Hf _{0.75} Nb _{0.25})B ₂ + Al ₂ Y + NbB
Hf	Y	Ta	-8.463426	-8.463306	-8.463852	-8.544402	-8.516465	-8.569082	106	106	105	25	53	Ta ₃ B ₄ + (Hf _{0.75} Ta _{0.25})B ₂ + (Ta _{0.5} Y _{0.5})B ₂ + Al ₂ Y + TaB
Hf	Y	Cr	-7.824193	-7.473053	-7.825348	N/A	N/A	-8.060478	236	587	235	N/A	N/A	Al ₃ Y + Cr₄AlB₄ + CrYB ₄ + Al ₂ Y + HfB ₂
Hf	Y	Mo	-8.062128	-8.063198	-8.062907	N/A	N/A	-8.276908	215	214	214	N/A	N/A	Mo₄AlB₄ + Mo_{4/3}Y_{2/3}AlB₂ + MoYB ₄ + MoAlB + HfB ₂
Hf	Y	W	-8.349757	-8.350570	-8.350447	N/A	N/A	-8.598295	249	248	248	N/A	N/A	W_{4/3}Y_{2/3}AlB₂ + YB ₄ + WB + WAlB + HfB ₂
Hf	Y	Mn	-7.712948	-7.711478	-7.711434	N/A	N/A	-7.971215	258	260	260	N/A	N/A	Mn_{4/3}Y_{2/3}AlB₂ + MnYB ₄ + Mn₂AlB₂ + HfB ₂
Hf	Y	Fe	-7.496015	-7.497162	-7.497007	N/A	N/A	-7.814901	319	318	318	N/A	N/A	Fe_{4/3}Y_{2/3}AlB₂ + Fe₂AlB₂ + FeYB ₄ + HfB ₂
V	Y	Sc	-7.372689	-7.371969	-7.371872	-7.381666	-7.331221	-7.423415	51	51	52	42	92	AlY ₂ + Al ₂ Y + VB + (Sc _{0.75} V _{0.25})B ₂
V	Y	Y	-7.228556	-7.227834	-7.228185	-7.182487	-7.201710	-7.290859	62	63	63	108	89	VYB ₄ + AlY ₂ + YB ₂ + Al ₂ Y
V	Y	Ti	-7.778783	-7.779150	-7.778969	-7.780539	-7.695065	-7.820935	42	42	42	40	126	(Ti _{0.75} V _{0.25})B ₂ + AlY ₂ + Al ₂ Y + VB
V	Y	Zr	-7.857967	-7.857919	-7.857896	-7.809834	-7.772062	-7.897974	40	40	40	88	126	V ₅ B ₆ + V ₃ B ₄ + (Zr _{0.75} Y _{0.25})B ₂ + Al ₂ Y + ZrB ₂
V	Y	Hf	-8.135471	-8.135514	-8.135489	-8.092398	-8.044527	-8.169866	34	34	34	77	125	V ₅ B ₆ + V ₃ B ₄ + (Hf _{0.75} Y _{0.25})B ₂ + Al ₂ Y + HfB ₂
V	Y	V	-7.840665	-7.840290	-7.839826	N/A	-7.777475	-7.863515	23	23	24	N/A	86	V ₂ B ₃ + VB ₂ + YB ₄ + Al ₂ Y
V	Y	Nb	-8.034106	-8.032900	-8.033155	-8.038298	-7.983741	-8.034503	0	2	1	-4	51	V ₂ B ₃ + (Nb _{0.75} Y _{0.25})B ₂ + (Nb_{0.83}Y_{0.17}) ₄ AlB₆ + Al ₃ Nb + Al ₂ Y
V	Y	Ta	-8.341974	-8.340815	-8.341135	-8.352199	-8.295843	-8.355666	14	15	15	3	60	(V _{0.5} Ta _{0.5}) ₂ B ₃ + TaYB ₄ + (Ta _{0.75} V _{0.25}) ₃ B ₄ + Al ₃ Y + YB ₄
V	Y	Cr	-7.738331	-7.738650	-7.739044	N/A	N/A	-7.868858	131	130	130	N/A	N/A	(V _{0.5} Cr _{0.5})B + (Cr _{0.75} V _{0.25})B + Al ₃ Y + Cr₂V₂AlB₆ + CrYB ₄
V	Y	Mo	-7.960421	-7.961656	-7.962065	N/A	N/A	-8.075135	115	113	113	N/A	N/A	MoAlB + (V _{0.5} Mo _{0.5})B + VB ₂ + MoYB ₄ + Mo_{4/3}Y_{2/3}AlB₂
V	Y	W	-8.248735	-8.251093	-8.251509	N/A	N/A	-8.408446	160	157	157	N/A	N/A	VB ₂ + YB ₄ + (W _{0.75} V _{0.25})B + Al ₅ W + (V _{0.5} W _{0.5})B
V	Y	Mn	-7.613302	-7.613714	-7.613527	N/A	N/A	-7.769934	157	157	156	N/A	N/A	Mn_{4/3}Y_{2/3}V₂AlB₆ + VB ₂ + MnYB ₄ + Mn₂AlB₂
V	Y	Fe	-7.400031	-7.401497	-7.401426	N/A	N/A	-7.613390	213	214	213	N/A	N/A	Fe₂VAlB₄ + Fe_{4/3}Y_{2/3}V₂AlB₆ + Fe₂AlB₂ + FeYB ₄
Nb	Y	Sc	-7.512739	-7.511730	-7.512016	-7.561563	-7.521235	-7.579010	66	67	67	17	58	(Sc _{0.75} Nb _{0.25})B ₂ + AlY ₂ + (Nb_{0.5}Sc_{0.5}) ₄ AlB₆ + Al ₂ Y + (Nb _{0.5} Sc _{0.5})B ₂
Nb	Y	Y	-7.385905	-7.385439	-7.385864	-7.393911	-7.396853	-7.424173	38	39	38	30	27	(Y _{0.75} Nb _{0.25})B ₂ + (Nb _{0.5} Y _{0.5})B ₂ + AlY ₂ + Al ₂ Y
Nb	Y	Ti	-7.895261	-7.894827	-7.894999	-7.917360	-7.857777	-7.938411	43	44	43	21	81	(Nb _{0.75} Ti _{0.25}) ₃ B ₄ + (Ti _{0.75} Nb _{0.25})B ₂ + AlY ₂ + Al ₂ Y
Nb	Y	Zr	-7.997621	-7.996782	-7.996962	-7.993194	-7.963734	-8.012052	14	15	15	19	48	(Zr _{0.75} Nb _{0.25})B ₂ + AlY ₂ + Al ₂ Y + NbB
Nb	Y	Hf	-8.270908	-8.270018	-8.270270	-8.266437	-8.232461	-8.286995	16	17	17	21	55	AlY ₂ + (Hf _{0.75} Nb _{0.25})B ₂ + Al ₂ Y + NbB
Nb	Y	V	-7.935111	-7.934810	-7.934316	-7.976403	-7.914033	-7.980591	45	46	46	4	67	(V _{0.75} Nb _{0.25})B ₂ + V ₂ B ₃ + Nb_{4/3}Y_{2/3}V₂AlB₆ + (Nb _{0.75} Y _{0.25})B ₂ + Al ₂ Y

Nb	Y	Nb	-8.142396	-8.142126	-8.141996	N/A	-8.145890	-8.142395	0	0	0	N/A	-3	(Nb _{0.78} Y _{0.22}) ₃ AlB ₄ + Nb ₂ B ₃ + (Nb _{0.75} Y _{0.25})B ₂ + Al ₃ Nb
Nb	Y	Ta	-8.446970	-8.446738	-8.446546	-8.484624	-8.451805	-8.482392	35	36	36	-2	31	(Ta _{0.75} Nb _{0.25}) ₂ B ₃ + Al ₃ Y + Ta _{4/3} Y _{2/3} NbAlB ₄ + Ta _{4/3} Y _{2/3} Nb ₂ AlB ₆ + YB ₄
Nb	Y	Cr	-7.821203	-7.821631	-7.824304	N/A	N/A	-7.971954	151	150	148	N/A	N/A	NbB ₂ + Cr _{4/3} Y _{2/3} Nb ₂ AlB ₆ + Cr ₂ AlB ₂ + CrYB ₄
Nb	Y	Mo	-8.052723	-7.675937	-8.054363	N/A	N/A	-8.192638	140	517	139	N/A	N/A	Mo ₂ Nb ₂ AlB ₆ + (Mo _{0.75} Nb _{0.25})B + Mo _{4/3} Y _{2/3} NbAlB ₄ + MoYB ₄ + MoAlB
Nb	Y	W	-8.337656	-8.339251	-8.340759	N/A	N/A	-8.513050	175	174	172	N/A	N/A	W _{4/3} Y _{2/3} Nb ₂ AlB ₆ + (W _{0.75} Nb _{0.25})B + YB ₄ + WAlB
Nb	Y	Mn	-7.707092	-7.707058	-7.706751	N/A	N/A	-7.885679	179	180	179	N/A	N/A	Mn _{4/3} Y _{2/3} Nb ₂ AlB ₆ + MnYB ₄ + Mn ₂ AlB ₂ + NbB ₂
Nb	Y	Fe	-7.494858	-7.494985	-7.495018	N/A	N/A	-7.726073	231	233	231	N/A	N/A	Fe _{4/3} Y _{2/3} Nb ₂ AlB ₆ + FeYB ₄ + NbB ₂ + Fe ₂ AlB ₂
Ta	Y	Sc	-7.722724	-7.721885	-7.722348	-7.775057	-7.732195	-7.798866	76	77	77	24	67	AlY ₂ + (Sc _{0.75} Ta _{0.25})B ₂ + TaB + Al ₂ Y
Ta	Y	Y	-7.595409	-7.594860	-7.595295	-7.600890	-7.604063	-7.632846	37	38	38	32	29	(Y _{0.75} Ta _{0.25})B ₂ + AlY ₂ + Al ₂ Y + TaB
Ta	Y	Ti	-8.104214	-8.104258	-8.104324	-8.130784	-8.070130	-8.158890	55	55	55	28	89	AlY ₂ + (Ti _{0.75} Ta _{0.25})B ₂ + Al ₂ Y + TaB
Ta	Y	Zr	-8.204872	-8.204089	-8.204360	-8.200224	-8.171471	-8.231031	26	27	27	31	60	(Zr _{0.75} Ta _{0.25})B ₂ + (Zr _{0.75} Y _{0.25})B ₂ + Al ₂ Y + TaB + ZrB ₂
Ta	Y	Hf	-8.477382	-8.476675	-8.476908	-8.472663	-8.439289	-8.503475	26	27	27	31	64	(Hf _{0.75} Y _{0.25})B ₂ + (Hf _{0.75} Ta _{0.25})B ₂ + Al ₂ Y + TaB + HfB ₂
Ta	Y	V	-8.143524	-8.143188	-8.142496	-8.188572	-8.123656	-8.194740	51	52	52	6	71	(V _{0.75} Ta _{0.25}) ₂ B ₃ + (V _{0.5} Ta _{0.5}) ₂ B ₃ + (Ta _{0.5} Y _{0.5})B ₂ + (V _{0.75} Ta _{0.25})B ₂ + Al ₂ Y
Ta	Y	Nb	-8.347024	-8.346660	-8.346149	-8.383142	-8.349911	-8.378948	32	32	33	-4	29	(Nb _{0.57} Ta _{0.43}) _{4/3} Y _{2/3} (Nb _{0.57} Ta _{0.43})AlB ₄ + (Nb _{0.5} Ta _{0.5}) ₂ B ₃ + (Nb _{0.75} Ta _{0.25})B ₂ + Al ₃ Nb + YB ₄
Ta	Y	Ta	-8.649561	-8.649127	-8.648759	N/A	-8.652509	-8.663778	14	15	15	N/A	11	Al ₄₃ Ta ₄ Y ₆ + Ta ₃ B ₄ + Al ₃ Y + YB ₄
Ta	Y	Cr	-8.029408	-8.029295	-8.032068	N/A	N/A	-8.175835	146	147	144	N/A	N/A	Cr ₂ AlB ₂ + (Ta _{0.75} Cr _{0.25})B ₂ + Cr _{4/3} Y _{2/3} Ta ₂ AlB ₆ + CrYB ₄
Ta	Y	Mo	-8.256517	-8.257335	-8.258283	N/A	N/A	-8.402423	146	146	145	N/A	N/A	Mo ₂ TaAlB ₄ + (Mo _{0.5} Ta _{0.5})B ₂ + MoYB ₄ + Mo _{4/3} Y _{2/3} TaAlB ₄
Ta	Y	W	-8.538555	-8.540699	-8.541930	N/A	N/A	-8.723752	185	183	182	N/A	N/A	(W _{0.5} Ta _{0.5})B ₂ + W _{4/3} Y _{2/3} TaAlB ₄ + YB ₄ + (W _{0.75} Ta _{0.25})B + Al ₅ W
Ta	Y	Mn	-7.915469	-7.916107	-7.915483	N/A	N/A	-8.090668	175	176	175	N/A	N/A	Mn _{4/3} Y _{2/3} Ta ₂ AlB ₆ + Mn ₂ AlB ₂ + MnYB ₄ + MnTaB ₃ + YB ₄
Ta	Y	Fe	-7.702922	-7.703454	-7.703791	N/A	N/A	-7.931009	228	230	227	N/A	N/A	Fe _{4/3} Y _{2/3} Ta ₂ AlB ₆ + FeTaB ₃ + Fe ₂ AlB ₂ + YB ₄ + FeYB ₄
Cr	Y	Sc	-7.382934	-7.382954	-7.382967	-7.337684	-7.299938	-7.407939	25	25	25	70	108	Cr ₄ AlB ₄ + CrYB ₄ + Al ₂ Y + CrB + ScB ₂
Cr	Y	Y	-7.235489	-7.235534	-7.235588	-7.137079	-7.174106	-7.324059	89	89	88	187	150	CrYB ₄ + YB ₂ + AlY ₂ + Al ₂ Y
Cr	Y	Ti	-7.785992	-7.786101	-7.785606	-7.730391	-7.643347	-7.810236	24	24	25	80	167	CrYB ₄ + CrB + Cr ₂ AlB ₄ + Al ₂ Y + TiB ₂
Cr	Y	Zr	-7.859197	-7.856503	-7.858253	-7.751140	-7.724531	-7.891717	33	35	33	141	167	CrYB ₄ + CrB + Cr ₂ AlB ₄ + Al ₂ Y + ZrB ₂
Cr	Y	Hf	-8.137440	-8.136691	-8.136543	-8.034124	-7.992508	-8.164636	27	28	28	131	172	Cr ₄ AlB ₄ + CrYB ₄ + Al ₂ Y + CrB + HfB ₂
Cr	Y	V	-7.854296	-7.854030	-7.853730	-7.837704	-7.727621	-7.870513	16	16	17	33	143	(V _{0.75} Cr _{0.25}) ₃ B ₄ + Al ₃ Y + Cr ₂ V ₂ AlB ₆ + CrYB ₄ + VB ₂
Cr	Y	Nb	-8.040794	-8.040226	-8.040470	-7.986730	-7.928757	-8.031220	-10	-9	-9	44	102	NbB ₂ + Cr _{4/3} Y _{2/3} NbAlB ₄
Cr	Y	Ta	-8.348710	-8.348077	-8.348403	-8.301180	-8.240082	-8.339123	-10	-9	-9	38	99	Ta ₂ B ₃ + Cr _{4/3} Y _{2/3} TaAlB ₄ + Al + Cr ₂ Ta ₂ AlB ₆ + CrYB ₄
Cr	Y	Cr	-7.758132	-7.760199	-7.759776	N/A	N/A	-7.825315	67	65	66	N/A	N/A	CrYB ₄ + Cr ₂ AlB ₂ + CrB ₄ + Cr ₄ AlB ₄
Cr	Y	Mo	-7.972927	-7.979290	-7.978911	N/A	N/A	-8.055681	83	76	77	N/A	N/A	(Mo _{0.5} Cr _{0.5})B + (Mo _{0.75} Cr _{0.25})B ₂ + CrYB ₄ + MoAlB
Cr	Y	W	-8.258671	-8.267931	-8.267683	N/A	N/A	-8.380219	122	112	113	N/A	N/A	(Cr _{0.5} W _{0.5})AlB + (W _{0.75} Cr _{0.25})B + (W _{0.75} Cr _{0.25})B ₂ + CrYB ₄ + WAlB
Cr	Y	Mn	-7.627509	-7.629478	-7.629050	N/A	N/A	-7.757357	130	128	128	N/A	N/A	CrYB ₄ + (Mn _{0.67} Cr _{0.33}) ₂ AlB ₂ + (Cr _{0.75} Mn _{0.25})B ₂ + MnYB ₄
Cr	Y	Fe	-7.410410	-7.406786	-7.412955	N/A	N/A	-7.587349	177	181	174	N/A	N/A	CrFe ₂ B ₄ + FeYB ₄ + (Cr _{0.75} Fe _{0.25})B ₄ + (Fe _{0.67} Cr _{0.33}) ₂ AlB ₂ + CrYB ₄
Mo	Y	Sc	-7.568273	-7.568351	-7.568305	-7.565953	-7.527650	-7.589758	21	21	21	24	62	AlMo ₃ + AlY ₂ + Al ₂ Y + Mo _{4/3} Y _{2/3} AlB ₂ + (Sc _{0.75} Mo _{0.25})B ₂
Mo	Y	Y	-7.431924	-7.432024	-7.432114	-7.381070	-7.401456	-7.443840	12	12	12	63	42	AlY ₂ + YB ₂ + MoYB ₄ + Al ₂ Y
Mo	Y	Ti	-7.948491	-7.948216	-7.947566	-7.913190	-7.850115	-7.966664	18	18	19	53	117	Mo _{4/3} Y _{2/3} AlB ₂ + TiB ₂
Mo	Y	Zr	-8.038624	-8.037644	-8.037344	-7.961935	-7.937189	-8.048145	10	11	11	86	111	Mo _{4/3} Y _{2/3} AlB ₂ + ZrB ₂
Mo	Y	Hf	-8.313684	-8.312562	-8.312310	-8.237959	-8.207499	-8.321064	7	9	9	83	114	Mo _{4/3} Y _{2/3} AlB ₂ + HfB ₂
Mo	Y	V	-7.996522	-7.996867	-7.998166	-7.986559	-7.908867	-8.010084	14	13	12	24	101	VB ₂ + Mo _{4/3} Y _{2/3} AlB ₂
Mo	Sc	Nb	-8.191803	-8.193530	-8.194202	-8.159250	-8.189692	-8.246573	55	53	52	87	57	Mo _{4/3} Y _{2/3} NbAlB ₄ + NbB ₂
Mo	Sc	Ta	-8.496978	-8.498704	-8.499224	-8.465324	-8.497455	-8.563075	66	64	64	98	66	Al ₂₂ Mo ₅ + Mo _{4/3} Y _{2/3} TaAlB ₄ + Ta ₃ B ₄ + (Ta _{0.75} Mo _{0.25})B ₂ + YB ₄
Mo	Sc	Cr	-7.897294	-7.898069	-7.897459	N/A	N/A	-7.994666	97	97	97	N/A	N/A	(Cr _{0.75} Mo _{0.25})B + Cr ₄ AlB ₄ + (Mo _{0.75} Cr _{0.25})B ₂ + CrYB ₄ + MoAlB
Mo	Sc	Mo	-8.108869	-8.114497	-8.113378	N/A	N/A	-8.208362	99	94	95	N/A	N/A	Mo ₃ YB ₇ + MoAlB + Mo ₄ AlB ₄
Mo	Sc	W	-8.391750	-8.398511	-8.397223	N/A	N/A	-8.565244	173	167	168	N/A	N/A	(Mo _{0.5} W _{0.5})AlB + (W _{0.75} Mo _{0.25})B + (Mo _{0.5} W _{0.5})B + YB ₄

Mo	Sc	Mn	-7.777586	-7.778714	-7.778775	N/A	N/A	-7.901750	124	123	123	N/A	N/A	MoB ₂ + (Mn_{0.67}Mo_{0.33})₂AlB₂ + MnYB ₄
Mo	Sc	Fe	-7.552469	-7.554054	-7.553810	N/A	N/A	-7.744324	192	190	191	N/A	N/A	FeYB ₄ + MoAlB + Mo ₃ YB ₇ + Fe₂AlB₂ + MoB ₂
W	Sc	Sc	-7.797503	-7.798093	-7.797946	-7.787760	-7.814325	-7.821531	24	23	24	34	7	ScW ₂ B ₄ + (Sc _{0.75} W _{0.25})B ₂ + WY ₃ B ₇ + Al ₂ Y + W
W	Sc	Y	-7.649513	-7.649836	-7.650012	-7.606215	-7.659712	-7.730669	81	81	81	124	71	W_{4/3}Y_{2/3}AlB₂ + WY ₃ B ₇ + YB ₄ + Al ₂ Y
W	Sc	Ti	-8.175792	-8.174661	-8.174303	-8.135276	-8.151388	-8.196517	21	22	22	61	45	W_{4/3}Y_{2/3}AlB₂ + TiB ₂
W	Sc	Zr	-8.250180	-8.249278	-8.248666	-8.168744	-8.210925	-8.280972	31	32	32	112	70	W_{4/3}Y_{2/3}AlB₂ + ZrB ₂
W	Sc	Hf	-8.526355	-8.525179	-8.524554	-8.444711	-8.484921	-8.559426	33	34	35	115	75	W_{4/3}Y_{2/3}AlB₂ + HfB ₂
W	Sc	V	-8.221999	-8.222997	-8.223955	-8.206591	-8.209920	-8.263664	42	41	40	57	54	VB ₂ + Al ₄₃ W ₄ Y ₆ + YB ₄ + Al ₃ Y + (V _{0.5} W _{0.5})B
W	Sc	Nb	-8.400847	-8.403392	-8.403887	-8.362028	-8.396530	-8.463412	63	60	60	101	67	W_{4/3}Y_{2/3}NbAlB₄ + NbB ₂
W	Sc	Ta	-8.703525	-8.706006	-8.706387	-8.662885	-8.699031	-8.775984	72	70	70	113	77	(Ta _{0.75} W _{0.25})B ₂ + W_{4/3}Y_{2/3}TaAlB₄ + YB ₄ + Al ₃ Y + (Ta _{0.75} W _{0.25})B
W	Sc	Cr	-8.108786	-8.109985	-8.109743	N/A	N/A	-8.212548	104	103	103	N/A	N/A	(Mo _{0.5} W _{0.5})B + (Cr_{0.5}W_{0.5})AlB + Cr₂AlB₂ + (W _{0.75} Cr _{0.25})B ₂ + CrYB ₄
W	Sc	Mo	-8.314618	-8.320070	-8.318891	N/A	N/A	-8.455004	140	135	136	N/A	N/A	(Mo_{0.5}W_{0.5})AlB + MoAlB + (Mo _{0.5} W _{0.5})B + YB ₄
W	Sc	W	-8.593764	-8.600278	-8.599201	N/A	N/A	-8.744329	151	144	145	N/A	N/A	WAlB + WB + YB ₄
W	Sc	Mn	-7.992526	-7.993597	-7.993858	N/A	N/A	-8.117781	125	124	124	N/A	N/A	(W _{0.75} Mn _{0.25})B + WB ₂ + Mn₂AlB₂ + MnYB ₄ + WAlB
W	Sc	Fe	-7.765105	-7.768538	-7.767285	N/A	N/A	-7.960355	195	192	193	N/A	N/A	WB ₂ + FeW ₂ B ₂ + WAlB + Fe₂AlB₂ + FeYB ₄
Mn	Sc	Sc	-7.350150	-7.350241	-7.350488	-7.254475	-7.274742	-7.374926	25	25	24	120	100	Mn_{4/3}Y_{2/3}AlB₂ + ScB ₂
Mn	Sc	Y	-7.188657	-7.187465	-7.188512	-7.070244	-7.149613	-7.289129	100	102	101	219	140	Mn_{4/3}Y_{2/3}AlB₂ + MnY ₃ B ₇ + MnYB ₄ + Al ₂ Y
Mn	Sc	Ti	-7.761595	-7.759651	-7.760022	-7.656179	-7.642428	-7.777223	16	18	17	121	135	Mn_{4/3}Y_{2/3}AlB₂ + TiB ₂
Mn	Sc	Zr	-7.818897	-7.816964	-7.817397	-7.669381	-7.697537	-7.871787	53	55	54	202	174	Mn_{4/3}Y_{2/3}AlB₂ + ZrB ₂
Mn	Sc	Hf	-8.099504	-8.097505	-8.097898	-7.952053	-7.974028	-8.141995	42	44	44	190	168	Mn_{4/3}Y_{2/3}AlB₂ + HfB ₂
Mn	Sc	V	-7.835076	-7.838152	-7.837360	-7.773725	-7.744512	-7.829973	-5	-8	-7	56	85	Mn_{4/3}Y_{2/3}VAlB₄ + VB ₂
Mn	Sc	Nb	-8.002636	-8.006781	-8.005956	-7.910978	-7.926213	-8.032196	30	25	26	121	106	Mn_{4/3}Y_{2/3}NbAlB₄ + NbB ₂
Mn	Sc	Ta	-8.310296	-8.314408	-8.313673	-8.225803	-8.241111	-8.344562	34	30	31	119	103	Mn_{4/3}Y_{2/3}TaAlB₄ + TaB ₂
Mn	Sc	Cr	-7.735013	-7.738567	-7.738579	N/A	N/A	-7.785256	50	47	47	N/A	N/A	CrYB ₄ + (Mn_{0.67}Cr_{0.33})₂AlB₂ + (Cr_{0.67}Mn_{0.33})₂AlB₂ + (Cr _{0.75} Mn _{0.25})B ₂
Mn	Sc	Mo	-7.938550	-7.941125	-7.941387	N/A	N/A	-8.004798	66	64	63	N/A	N/A	MoB ₂ + (Mo_{0.67}Mn_{0.33})₂AlB₂ + MnYB ₄
Mn	Sc	W	-8.226319	-8.229667	-8.230077	N/A	N/A	-8.327139	101	97	97	N/A	N/A	(W _{0.75} Mn _{0.25})B + WB ₂ + Mn₂AlB₂ + MnYB ₄ + WAlB
Mn	Sc	Mn	-7.605835	-7.610484	-7.607357	N/A	N/A	-7.648654	43	38	41	N/A	N/A	Mn₄AlB₄ + MnB ₄ + Mn₂AlB₂ + MnYB ₄
Mn	Sc	Fe	-7.380371	-7.377787	-7.377804	N/A	N/A	-7.506470	126	129	129	N/A	N/A	(Fe_{0.67}Mn_{0.33})₂AlB₂ + MnB ₄ + FeB + MnYB ₄ + FeYB ₄
Fe	Sc	Sc	-7.254235	-7.254246	-7.254296	-7.116718	-7.144841	-7.270740	17	16	16	154	126	Fe_{4/3}Y_{2/3}AlB₂ + ScB ₂
Fe	Sc	Y	-7.093553	-7.093529	-7.093548	-6.956191	-7.029529	-7.188030	94	95	94	232	159	FeY ₃ B ₇ + Fe ₂ YB ₂ + FeYB ₄ + Al ₂ Y
Fe	Sc	Ti	-7.654632	-7.447912	-7.653448	-7.514636	-7.502540	-7.677636	23	230	24	163	175	Fe_{4/3}Y_{2/3}AlB₂ + TiB ₂
Fe	Sc	Zr	-7.706554	-7.706081	-7.706233	-7.526654	-7.563587	-7.773124	67	67	67	246	210	Fe_{4/3}Y_{2/3}AlB₂ + ZrB ₂
Fe	Sc	Hf	-7.987936	-7.987397	-7.987484	-7.808814	-7.835100	-8.051577	64	64	64	243	216	Fe_{4/3}Y_{2/3}AlB₂ + HfB ₂
Fe	Sc	V	-7.729959	-7.729084	-7.733091	-7.638676	-7.604097	-7.727093	-3	1	-3	88	123	Fe_{4/3}Y_{2/3}VAlB₄ + VB ₂
Fe	Sc	Nb	-7.896193	-7.900146	-7.899599	-7.769378	-7.783138	-7.937326	41	37	38	168	154	Fe_{4/3}Y_{2/3}NbAlB₄ + NbB ₂
Fe	Sc	Ta	-8.204978	-8.209034	-8.208435	-8.085034	-8.098868	-8.244383	39	35	36	159	146	Fe_{4/3}Y_{2/3}TaAlB₄ + TaB ₂
Fe	Sc	Cr	-7.614890	-7.615745	-7.615916	N/A	N/A	-7.667060	52	51	51	N/A	N/A	CrB ₄ + (Fe_{0.67}Cr_{0.33})₂AlB₂ + CrYB ₄ + CrB
Fe	Sc	Mo	-7.822403	-7.818742	-7.819646	N/A	N/A	-7.899003	77	80	79	N/A	N/A	FeYB ₄ + MoAlB + Mo ₃ YB ₇ + Fe₂AlB₂ + MoB ₂
Fe	Sc	W	-8.114063	-8.108596	-8.110535	N/A	N/A	-8.221729	108	113	111	N/A	N/A	WB ₂ + FeW ₂ B ₂ + WAlB + Fe₂AlB₂ + FeYB ₄
Fe	Sc	Mn	-7.493631	-7.493676	-7.493594	N/A	N/A	-7.558666	65	65	65	N/A	N/A	(Fe_{0.67}Mn_{0.33})₂AlB₂ + MnB ₄ + FeB + MnYB ₄ + (Mn_{0.67}Fe_{0.33})₂AlB₂
Fe	Sc	Fe	-7.258485	-7.252892	-7.256910	N/A	N/A	-7.365248	107	112	108	N/A	N/A	Fe₂AlB₂ + YB ₄ + FeB

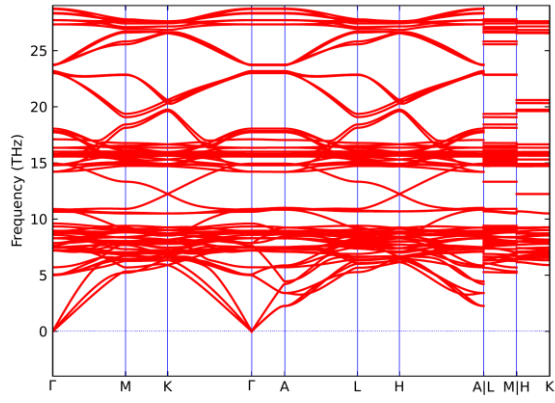


Figure S3. Phonon dispersion spectra for 314 *s*-MAB phase $\text{Mn}_{4/3}\text{Sc}_{2/3}\text{VAlB}_4$.

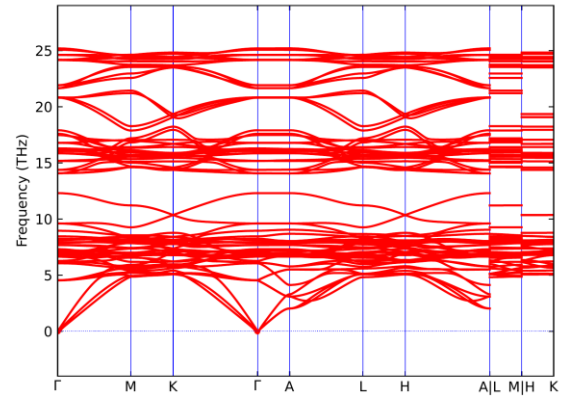


Figure S6. Phonon dispersion spectra for 314 *s*-MAB phase $\text{Cr}_{4/3}\text{Y}_{2/3}\text{NbAlB}_4$.

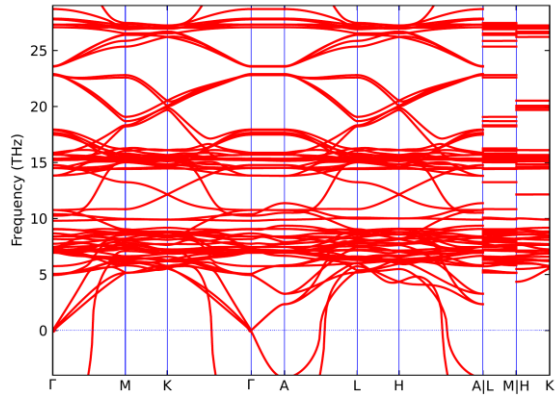


Figure S4. Phonon dispersion spectra for 314 *s*-MAB phase $\text{Fe}_{4/3}\text{Sc}_{2/3}\text{VAlB}_4$.

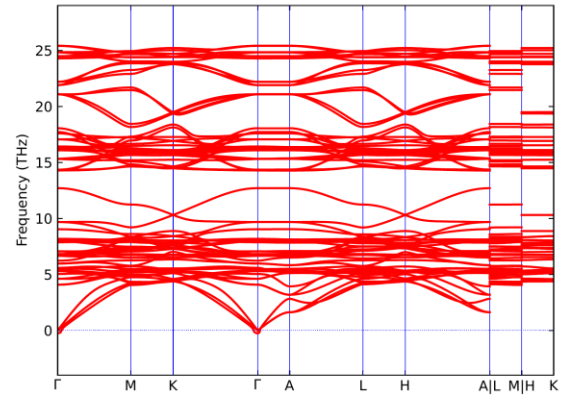


Figure S7. Phonon dispersion spectra for 314 *s*-MAB phase $\text{Cr}_{4/3}\text{Y}_{2/3}\text{TaAlB}_4$.

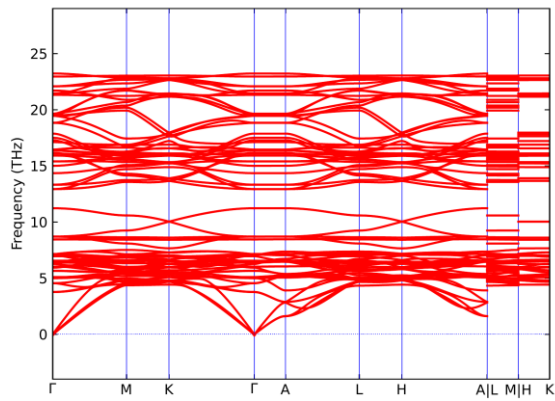


Figure S5. Phonon dispersion spectra for 314 *s*-MAB phase $\text{Nb}_{4/3}\text{Y}_{2/3}\text{NbAlB}_4$.

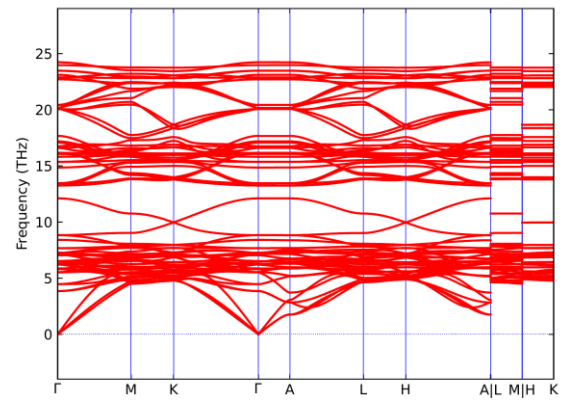


Figure S8. Phonon dispersion spectra for 314 *s*-MAB phase $\text{Mo}_{4/3}\text{Y}_{2/3}\text{NbAlB}_4$.

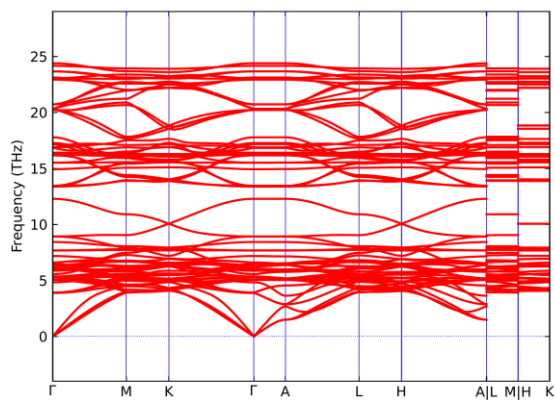


Figure S9. Phonon dispersion spectra for 314 *s*-MAB phase $\text{Mo}_{4/3}\text{Y}_{2/3}\text{TaAlB}_4$.

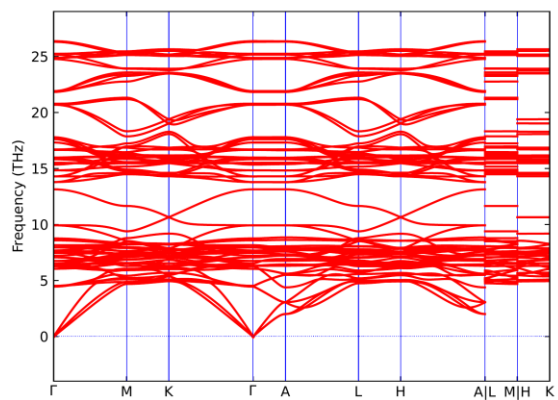


Figure S12. Phonon dispersion spectra for 314 *s*-MAB phase $\text{Mn}_{4/3}\text{Y}_{2/3}\text{NbAlB}_4$.

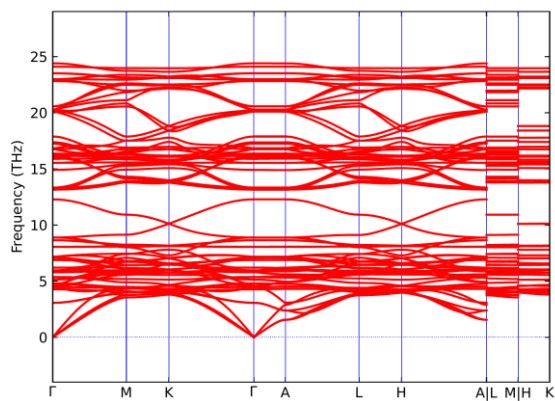


Figure S10. Phonon dispersion spectra for 314 *s*-MAB phase $\text{W}_{4/3}\text{Y}_{2/3}\text{NbAlB}_4$.

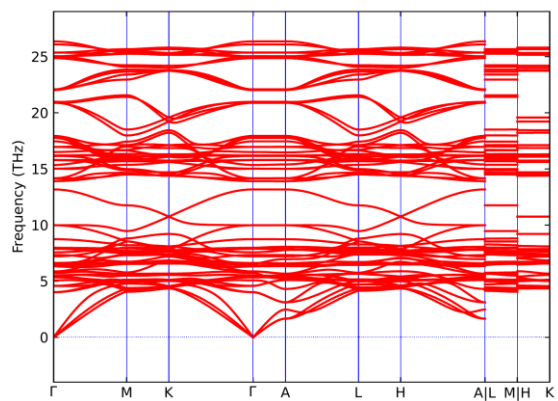


Figure S13. Phonon dispersion spectra for 314 *s*-MAB phase $\text{Mn}_{4/3}\text{Y}_{2/3}\text{TaAlB}_4$.

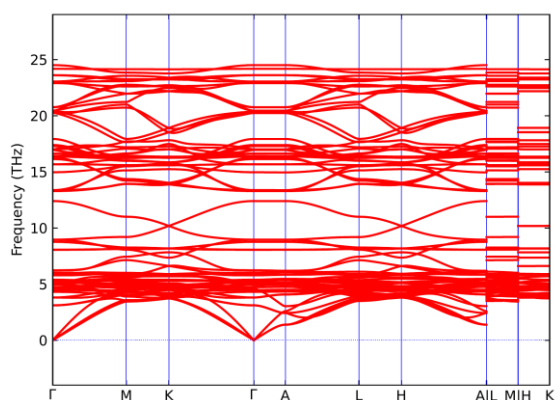


Figure S11. Phonon dispersion spectra for 314 *s*-MAB phase $\text{W}_{4/3}\text{Y}_{2/3}\text{TaAlB}_4$.

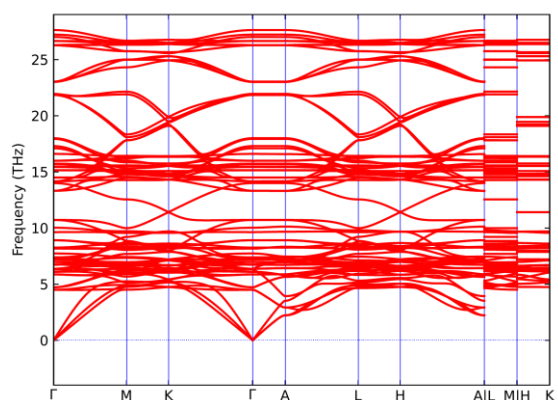


Figure S14. Phonon dispersion spectra for 314 *s*-MAB phase $\text{Fe}_{4/3}\text{Y}_{2/3}\text{VAlB}_4$.

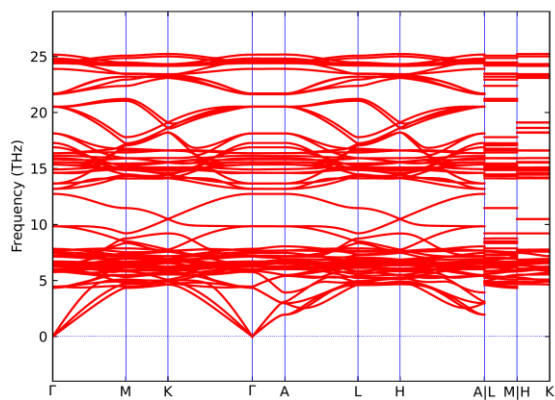


Figure S15. Phonon dispersion spectra for 314 *s*-MAB phase $\text{Fe}_{4/3}\text{Y}_{2/3}\text{NbAlB}_4$.

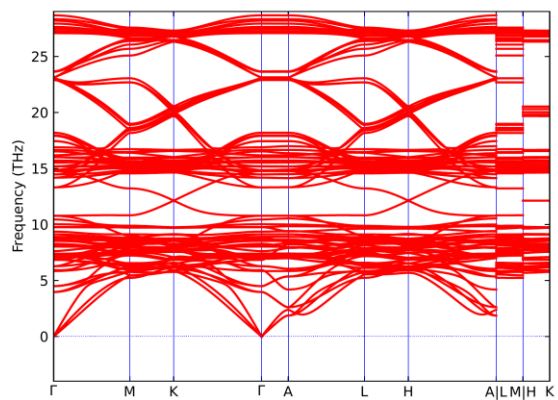


Figure S18. Phonon dispersion spectra for 416 *s*-MAB phase $\text{Fe}_{4/3}\text{Sc}_{2/3}\text{V}_2\text{AlB}_6$.

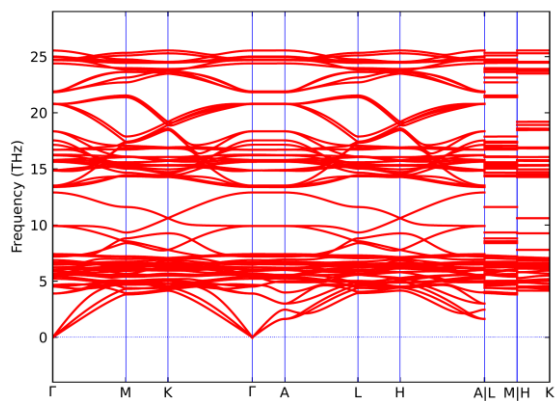


Figure S16. Phonon dispersion spectra for 314 *s*-MAB phase $\text{Fe}_{4/3}\text{Y}_{2/3}\text{TaAlB}_4$.

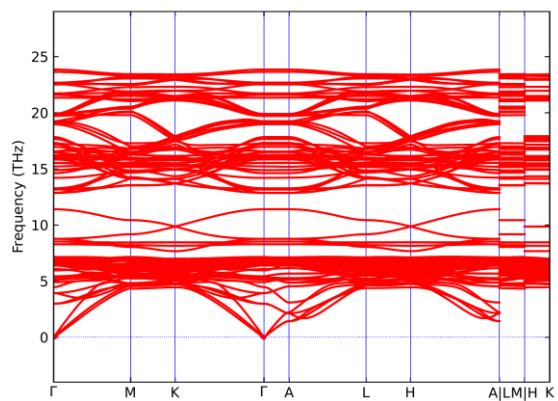


Figure S19. Phonon dispersion spectra for 416 *s*-MAB phase $(\text{Nb}_{2/3}\text{Y}_{2/3}\text{Nb}_2)\text{AlB}_6$.

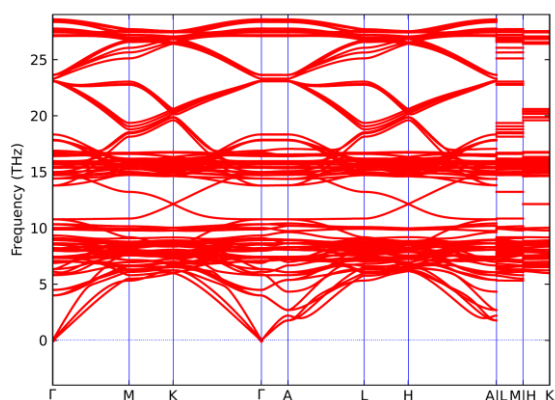


Figure S17. Phonon dispersion spectra for 416 *s*-MAB phase $\text{Mn}_{4/3}\text{Sc}_{2/3}\text{V}_2\text{AlB}_6$.

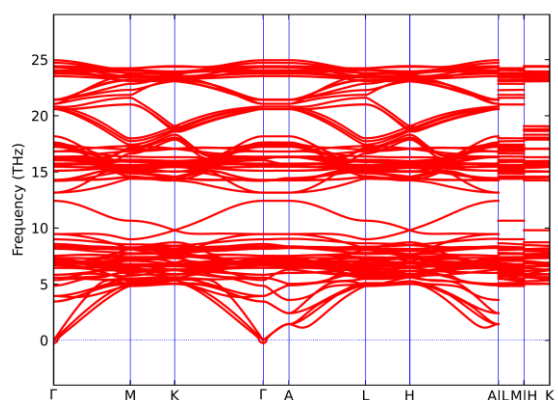


Figure S20. Phonon dispersion spectra for 416 *s*-MAB phase $\text{Cr}_{4/3}\text{Y}_{2/3}\text{Nb}_2\text{AlB}_6$.

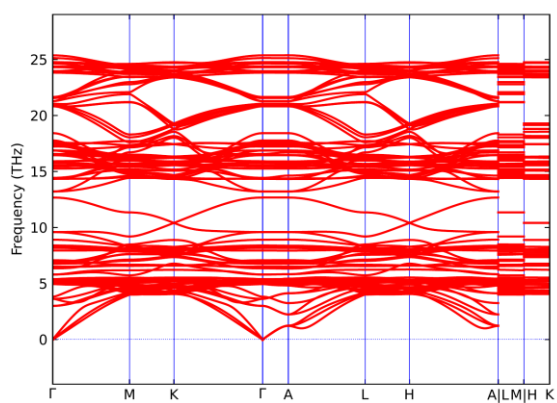


Figure S21. Phonon dispersion spectra for 416 *s*-MAB phase $\text{Cr}_{4/3}\text{Y}_{2/3}\text{Ta}_2\text{AlB}_6$.

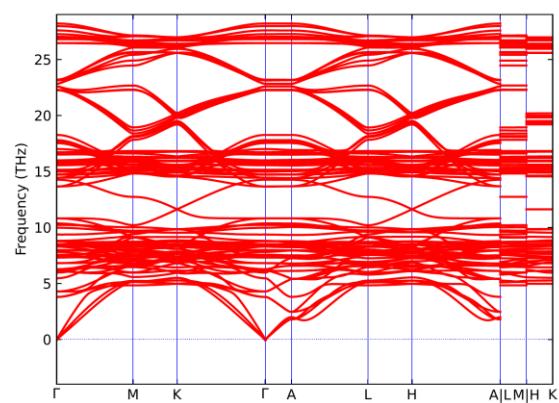


Figure S24. Phonon dispersion spectra for 416 *s*-MAB phase $\text{Mn}_{4/3}\text{Y}_{2/3}\text{V}_2\text{AlB}_6$.

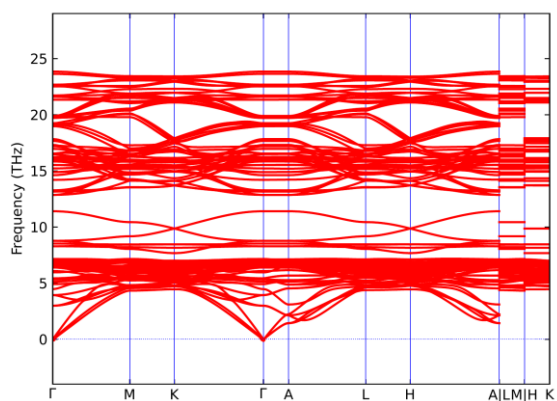


Figure S22. Phonon dispersion spectra for 416 *s*-MAB phase $\text{Mo}_{4/3}\text{Y}_{2/3}\text{Nb}_2\text{AlB}_6$.

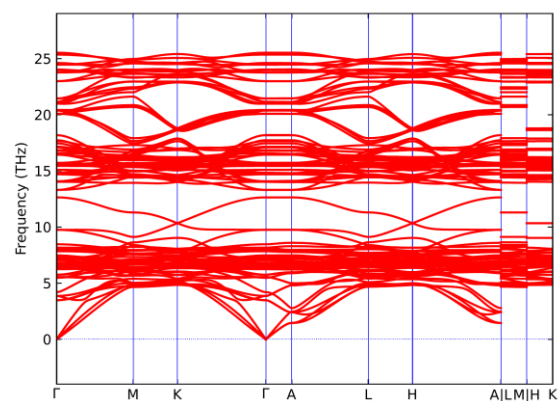


Figure S25. Phonon dispersion spectra for 416 *s*-MAB phase $\text{Mn}_{4/3}\text{Y}_{2/3}\text{Nb}_2\text{AlB}_6$.

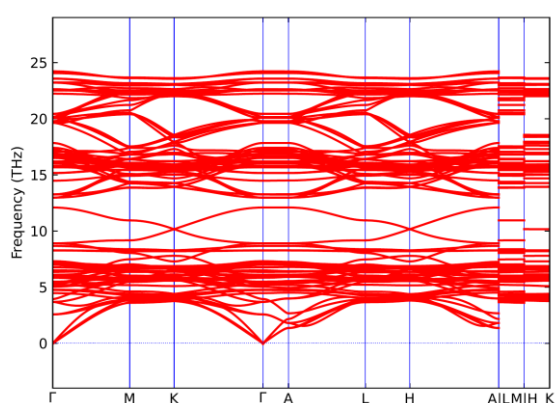


Figure S23. Phonon dispersion spectra for 416 *s*-MAB phase $\text{W}_{4/3}\text{Y}_{2/3}\text{Nb}_2\text{AlB}_6$.

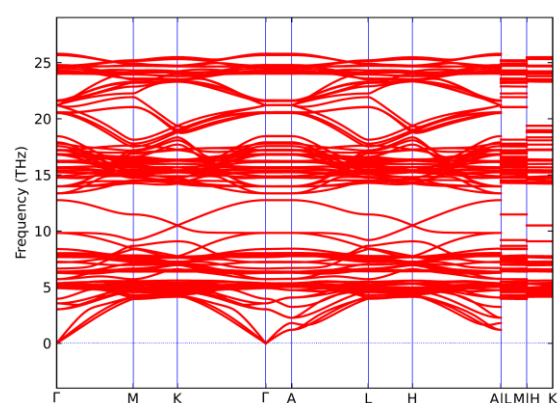


Figure S26. Phonon dispersion spectra for 416 *s*-MAB phase $\text{Mn}_{4/3}\text{Y}_{2/3}\text{Ta}_2\text{AlB}_6$.

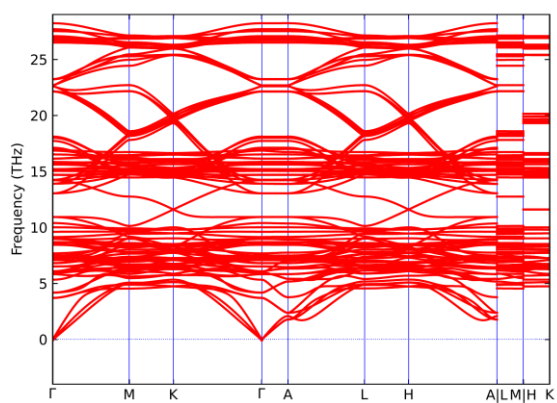


Figure S27. Phonon dispersion spectra for 416 *s*-MAB phase $\text{Fe}_{4/3}\text{Y}_{2/3}\text{V}_2\text{AlB}_6$.

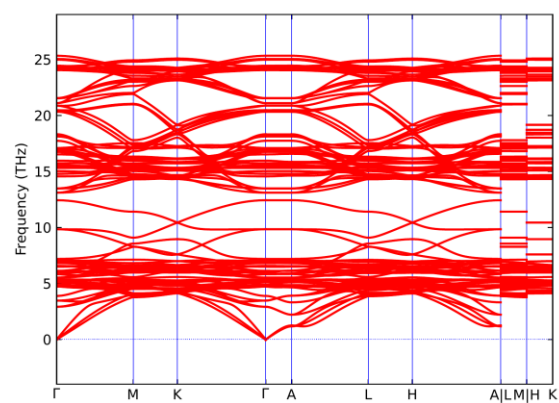


Figure S29. Phonon dispersion spectra for 416 *s*-MAB phase $\text{Fe}_{4/3}\text{Y}_{2/3}\text{Ta}_2\text{AlB}_6$.

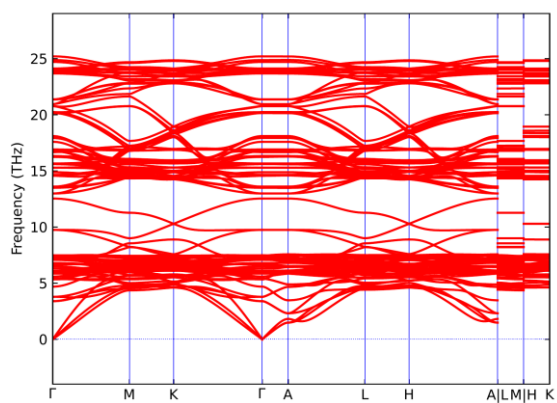


Figure S28. Phonon dispersion spectra for 416 *s*-MAB phase $\text{Fe}_{4/3}\text{Y}_{2/3}\text{Nb}_2\text{AlB}_6$.

Table S6. Calculated structural data for $\text{Mo}_{4/3}\text{Y}_{2/3}\text{Nb}_2\text{AlB}_6$ *s*-MAB in structures with $P6/mmm$, $P6_3/mmc$, and $R-3m$ space group symmetry. Structural relaxation performed using GGA-PBE exchange-correlation functional. Note that data for $R-3m$ is given in its hexagonal representation.

<i>s</i> -MAB	Space group	Lattice parameters	Wyckoff site
$\text{Mo}_{4/3}\text{Y}_{2/3}\text{Nb}_2\text{AlB}_6$	$P6/mmm$ no. 191	$a = b = 5.43621 \text{ \AA}$ $c = 14.2269 \text{ \AA}$ $\alpha = \beta = 90^\circ$ $\gamma = 120^\circ$	Mo1: 4h (0.33333, 0.66667, 0.83203) Y1: 2e (0.00000, 0.00000, 0.87496) Nb1: 4h (0.33333, 0.66667, 0.61489) Nb2: 2e (0.00000, 0.00000, 0.61661) Al1: 3f (0.50000, 0.00000, 0.00000) B1: 12n (0.66795, 0.00000, 0.73470) B2: 6k (0.66565, 0.00000, 0.50000)
$\text{Mo}_{4/3}\text{Y}_{2/3}\text{Nb}_2\text{AlB}_6$	$P6_3/mmc$ no. 194	$a = b = 5.43057 \text{ \AA}$ $c = 28.4968 \text{ \AA}$ $\alpha = \beta = 90^\circ$ $\gamma = 120^\circ$	Mo1: 4e (0.00000, 0.00000, 0.83365) Mo2: 4f (0.33333, 0.66667, 0.83362) Y1: 4f (0.33333, 0.66667, 0.31303) Nb1: 4e (0.00000, 0.00000, -0.05761) Nb2: 4f (0.33333, 0.66667, -0.05759) Nb3: 4f (0.33333, 0.66667, 0.44162) Al1: 6h (0.83368, 0.66737, 0.25000) B1: 24l (-0.00091, 0.33365, 0.88272) B2: 12i (0.33295, 0.00000, 0.00000)
$\text{Mo}_{4/3}\text{Y}_{2/3}\text{Nb}_2\text{AlB}_6$	$R-3m$ (hexagonal axes) no. 166	$a = b = 5.43288 \text{ \AA}$ $c = 42.7094 \text{ \AA}$ $\alpha = \beta = 90^\circ$ $\gamma = 120^\circ$	Mo1: 6c (0.00000, 0.00000, 0.61087) Mo2: 6c (0.00000, 0.00000, 0.27746) Y1: 6c (0.00000, 0.00000, -0.04202) Nb1: 6c (0.00000, 0.00000, 0.87228) Nb2: 6c (0.00000, 0.00000, 0.53845) Nb3: 6c (0.00000, 0.00000, 0.20501) Al1: 9e (0.50000, 0.00000, 0.00000) B1: 36i (0.33443, 0.00129, 0.24485) B2: 18g (0.33287, 0.00000, 0.50000)

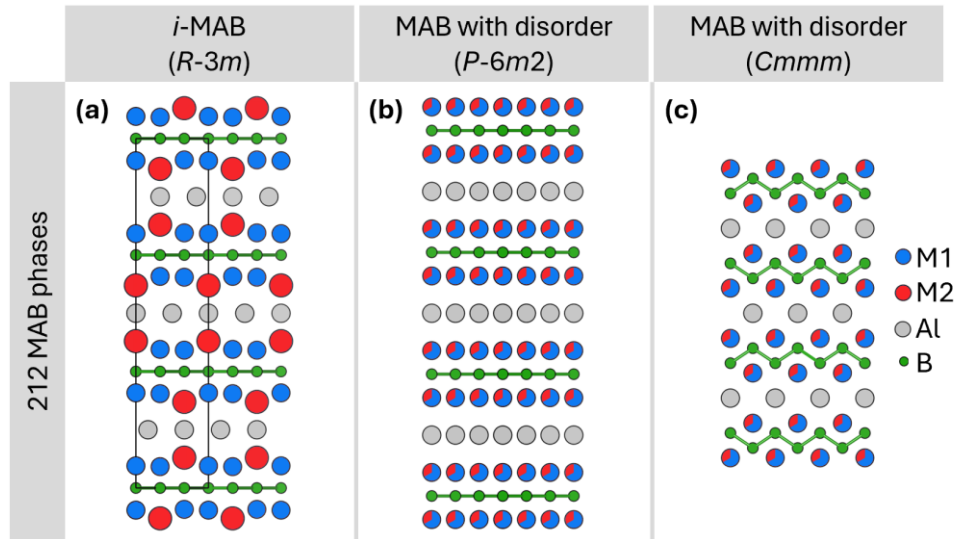


Figure S30. Schematic illustration of different distribution of metals M1 and M2 in 212 MAB phases. (a) *i*-MAB phase with in-plane order with space group symmetry $R-3m$, disorder of M1 and M2 across all metal layers in MAB phase with space group symmetry (b) $P-6m2$ and (c) $Cmmm$.

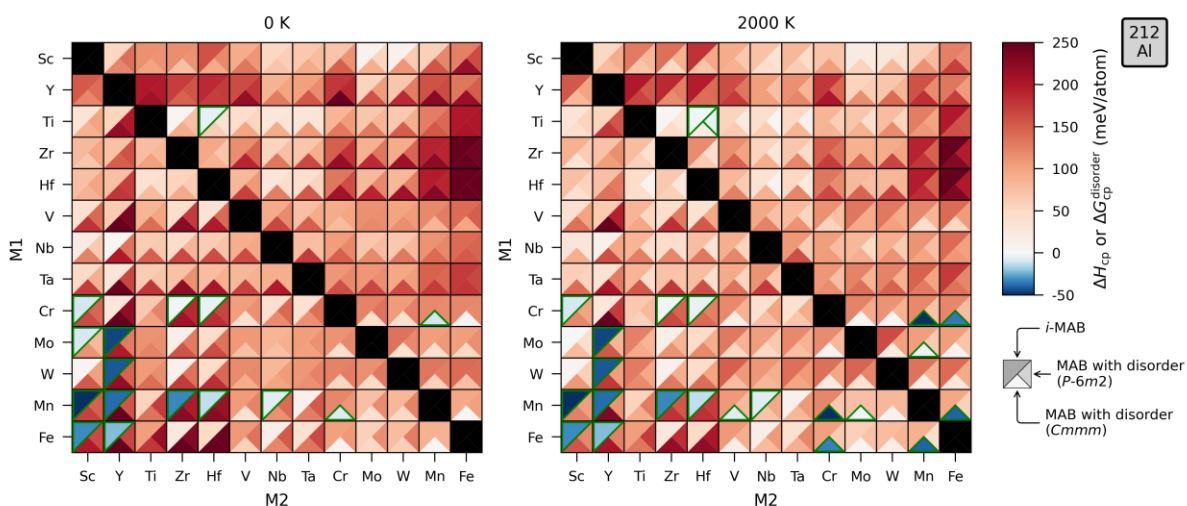


Figure S31. Stability heatmap for quaternary 212 MAB phases at (a) 0 K and (b) 2000 K upon mixing metals M1 and M2 in a 2:1 ratio with coloring representing calculated stability. For a given combination of M1 and M2, the upper left triangles represent in-plane ordered *i*-MAB, right triangles represent hexagonal MAB, space group $P-6m2$, with disorder of M1 and M2, and bottom triangles represent orthorhombic MAB, space group $Cmmm$, with disorder of M1 and M2. Stable phases are framed in green. Black triangles represent combinations of M1 and M2 not considered.

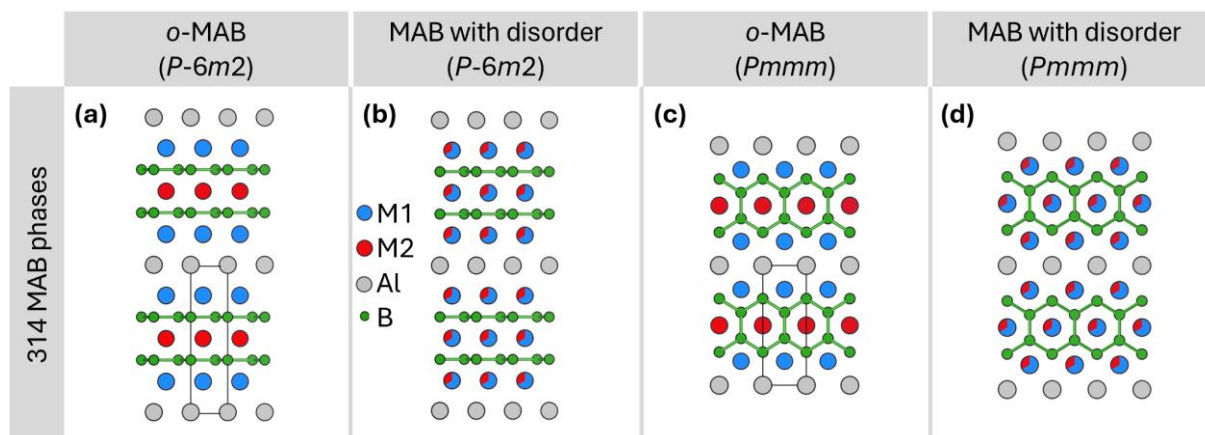


Figure S32. Schematic illustration of different distribution of metals M1 and M2 in 314 MAB phases. *o*-MAB phase with out-of-plane order with space group symmetry (a) $P-6m2$ and (c) $Pmmm$. Disorder of M1 and M2 across all metal layers in MAB phase with space group symmetry (b) $P-6m2$ and (d) $Pmmm$.

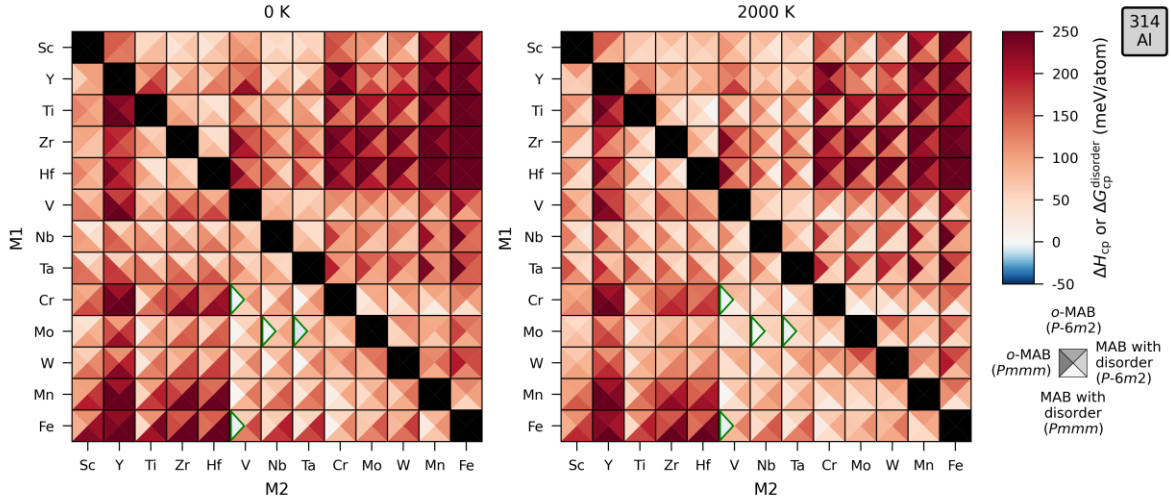


Figure S33. Stability heatmap for quaternary 314 MAB phases at (a) 0 K and (b) 2000 K upon mixing metals M1 and M2 in a 2:1 ratio with coloring representing calculated stability. For a given combination of M1 and M2, the upper triangles represent out-of-plane ordered *o*-MAB in space group *P-6m2*, left triangles represent out-of-plane ordered *o*-MAB in space group *Pmmm*, right triangles represent hexagonal MAB, space group *P-6m2*, with disorder of M1 and M2, and bottom triangles represent orthorhombic MAB, space group *Pmmm*, with disorder of M1 and M2. Stable phases are framed in green. Black triangles represent combinations of M1 and M2 not considered.

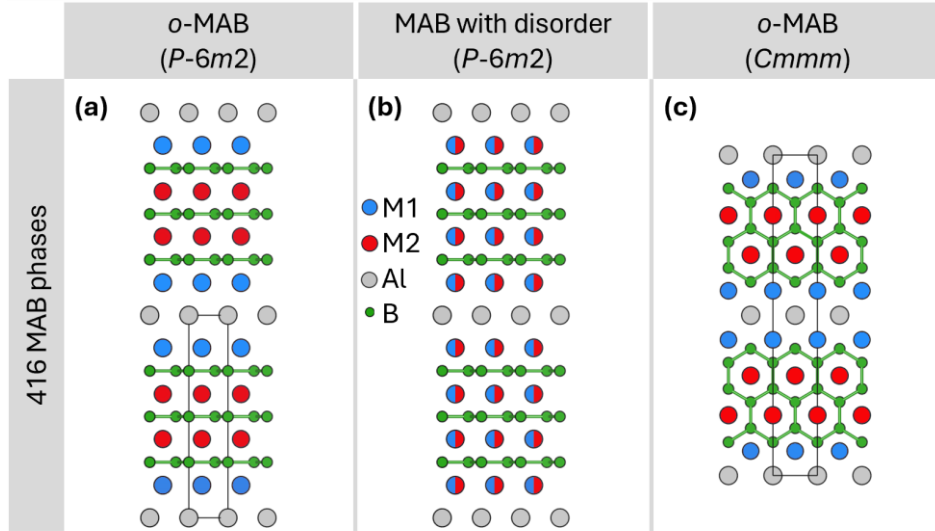


Figure S34. Schematic illustration of different distribution of metals M1 and M2 in 416 MAB phases. *o*-MAB phase with out-of-plane order with space group symmetry (a) *P-6m2* and (c) *Cmmm*. Disorder of M1 and M2 across all metal layers in MAB phase with space group symmetry (b) *P-6m2*.

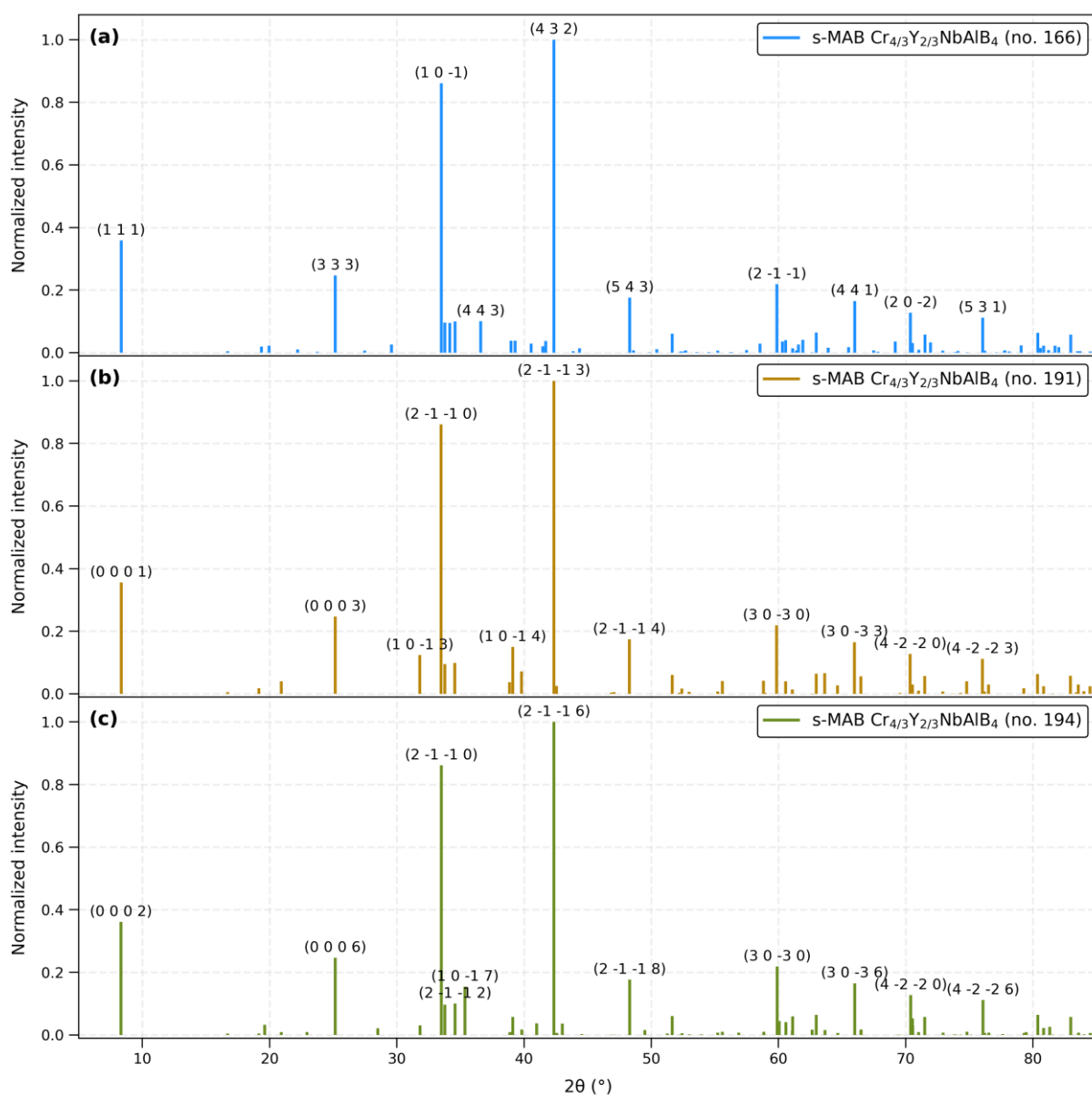


Figure S36. Simulated XRD using Cu-K α for Cr $_{4/3}$ Y $_{2/3}$ NbAlB $_4$ s-MAB structure in space group (a) $R\bar{3}m$ (no. 166), (b) $P6/mmm$ (no. 191), and (c) $P6_3/mmc$ (no. 194). Peak notation given for peaks with at least 10% intensity relative to the maximum peak. Note that peak notation for no. 166 is based on the rhombohedral structure.

Table S7. EDX on four particles for sample with nominal Cr $_{4/3}$ Y $_{2/3}$ NbAlB $_4$ composition.

Particle	Cr at%	Y at%	Nb at%	Al at%	B at%	C at%	O at%	Cr/Y	Cr/Nb	(Cr+Y+Nb)/Y	(Cr+Y+Nb)/Al
1	8.7	5	8.3	6	54.6	16.3	1.1	1.74	1.05	4.40	3.67
2	9	5.1	7.9	6.2	59.6	10.4	1.8	1.76	1.14	4.31	3.55
3	10.6	6.3	8.9	8.6	57.9	5.9	1.8	1.68	1.19	4.10	3.00
4	9.3	5.6	7.7	7.5	63	6.3	0.6	1.66	1.21	4.04	3.01
SD	0.7	0.5	0.5	1.1	3	4.2	0.5	0.05	0.07	0.17	0.35
Average	9.4	5.5	8.2	7.1	58.8	9.7	1.3	1.71	1.15	4.20	3.27

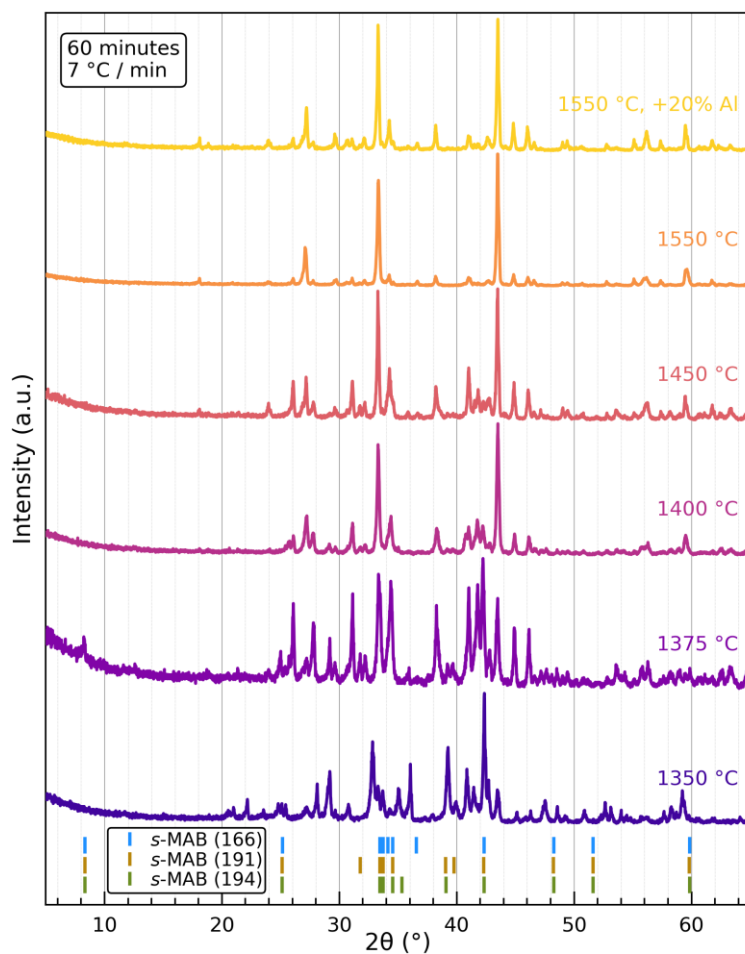


Figure S37. XRD diffractograms for samples with various sintering temperatures with a reaction time of 60 minutes and a ramping rate of 7 °C/min.

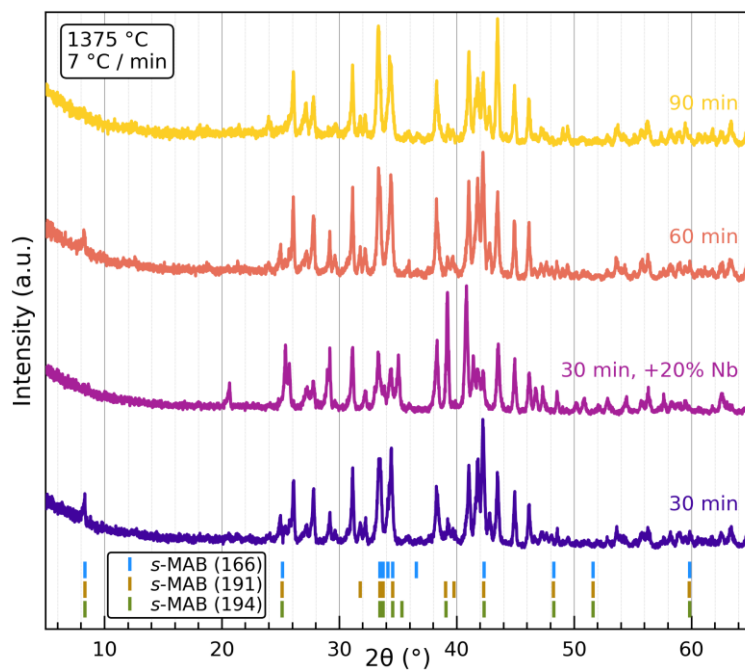


Figure S38. XRD diffractograms for samples with various reaction times at a sintering temperature of 1375 °C and a ramping rate of 7 °C/min.

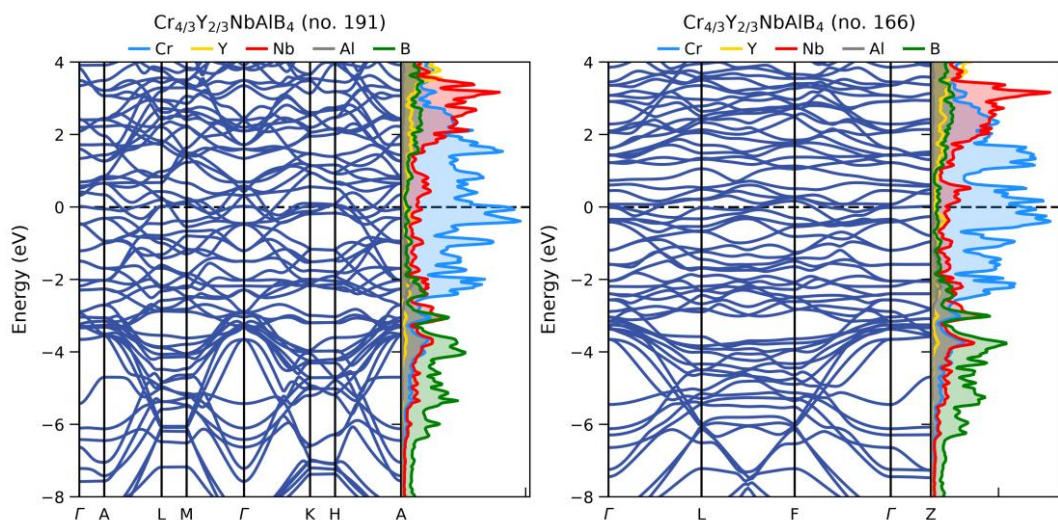


Figure S39. Calculated electronic band-structure and density of states for $\text{Cr}_{4/3}\text{Y}_{2/3}\text{NbAlB}_4$ *s*-MAB phase with $P6/mmm$ and $R-3m$ space group symmetry.

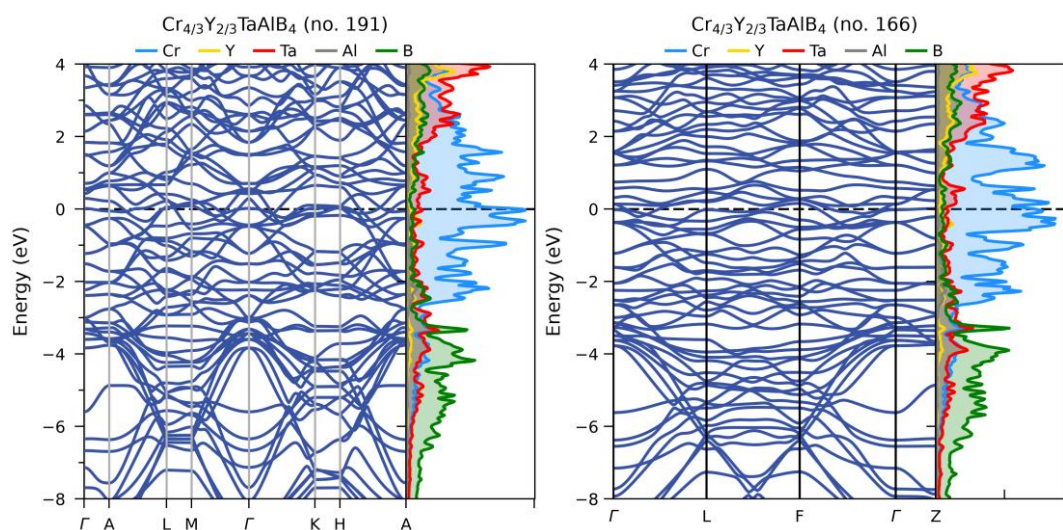


Figure S40. Calculated electronic band-structure and density of states for $\text{Cr}_{4/3}\text{Y}_{2/3}\text{TaAlB}_4$ *s*-MAB phase with $P6/mmm$ and $R-3m$ space group symmetry.

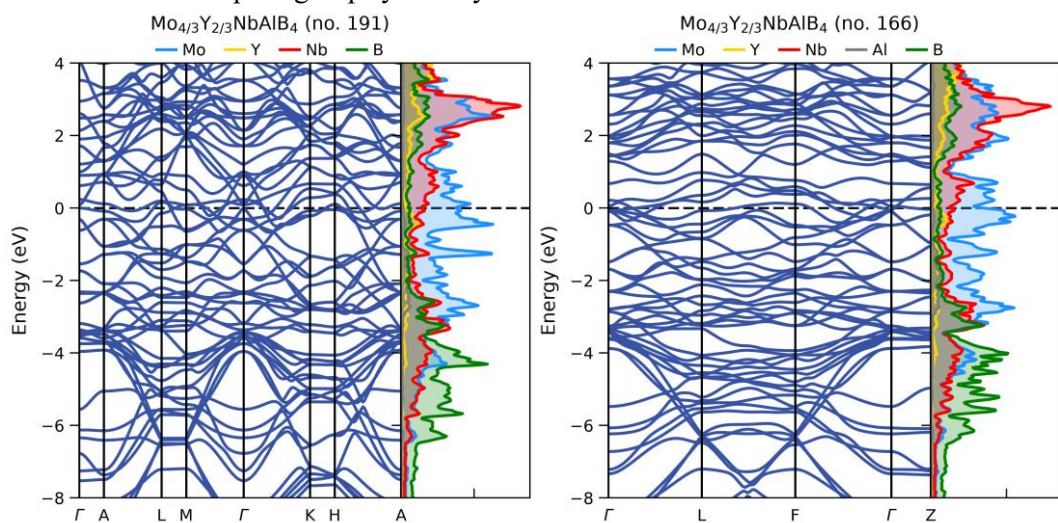


Figure S41. Calculated electronic band-structure and density of states for $\text{Mo}_{4/3}\text{Y}_{2/3}\text{NbAlB}_4$ *s*-MAB phase with $P6/mmm$ and $R-3m$ space group symmetry.

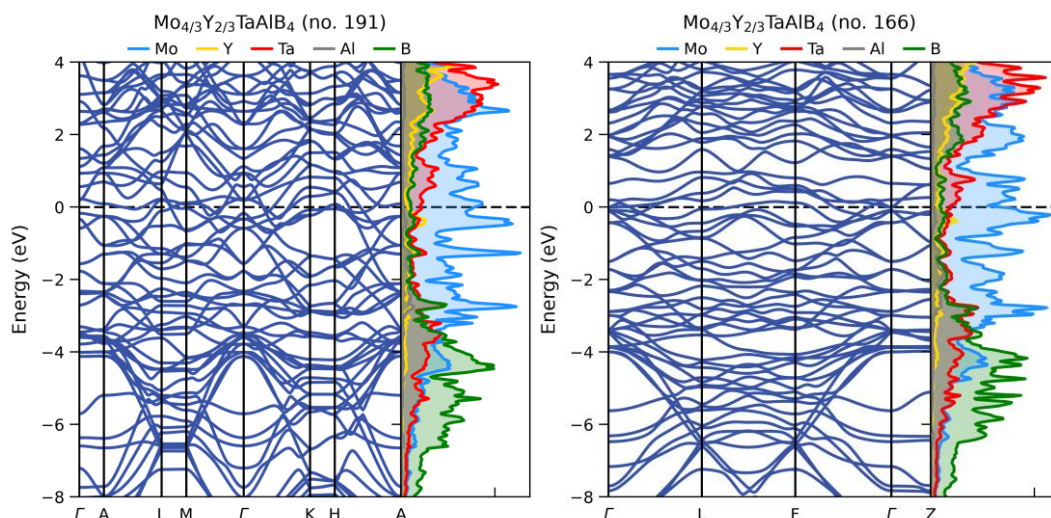


Figure S42. Calculated electronic band-structure and density of states for $\text{Mo}_{4/3}\text{Y}_{2/3}\text{TaAlB}_4$ *s*-MAB phase with $P6/mmm$ and $R\bar{3}m$ space group symmetry.

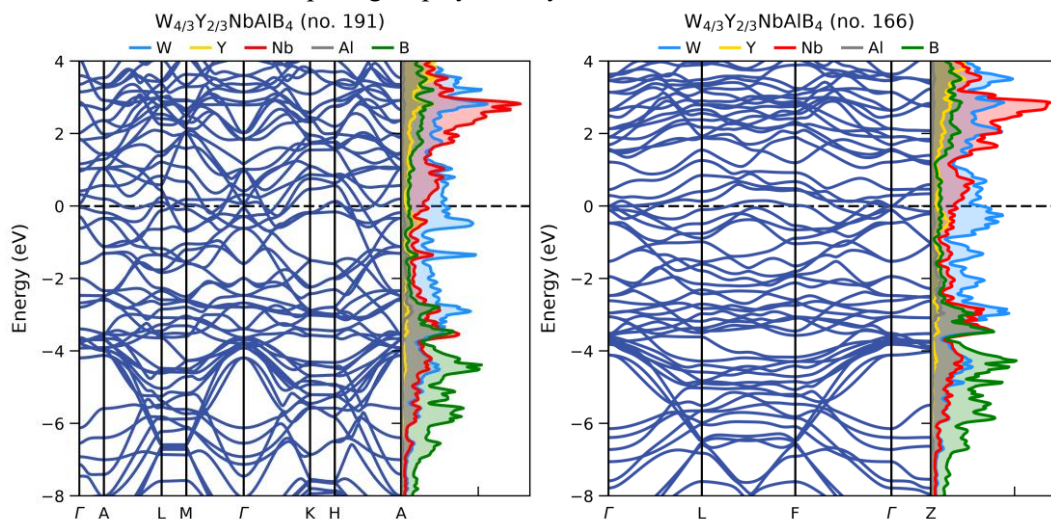


Figure S43. Calculated electronic band-structure and density of states for $\text{W}_{4/3}\text{Y}_{2/3}\text{NbAlB}_4$ *s*-MAB phase with $P6/mmm$ and $R\bar{3}m$ space group symmetry.

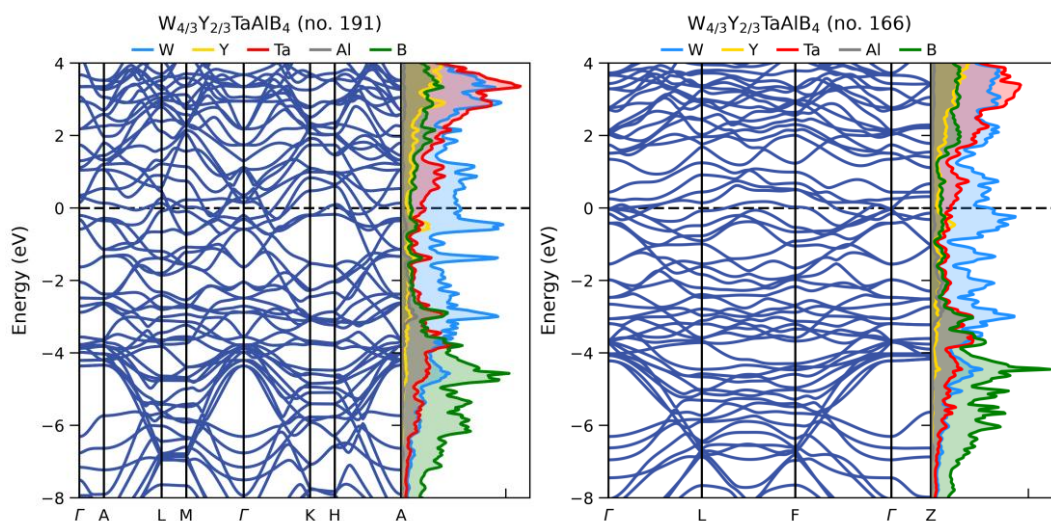


Figure S44. Calculated electronic band-structure and density of states for $\text{W}_{4/3}\text{Y}_{2/3}\text{TaAlB}_4$ *s*-MAB phase with $P6/mmm$ and $R\bar{3}m$ space group symmetry.

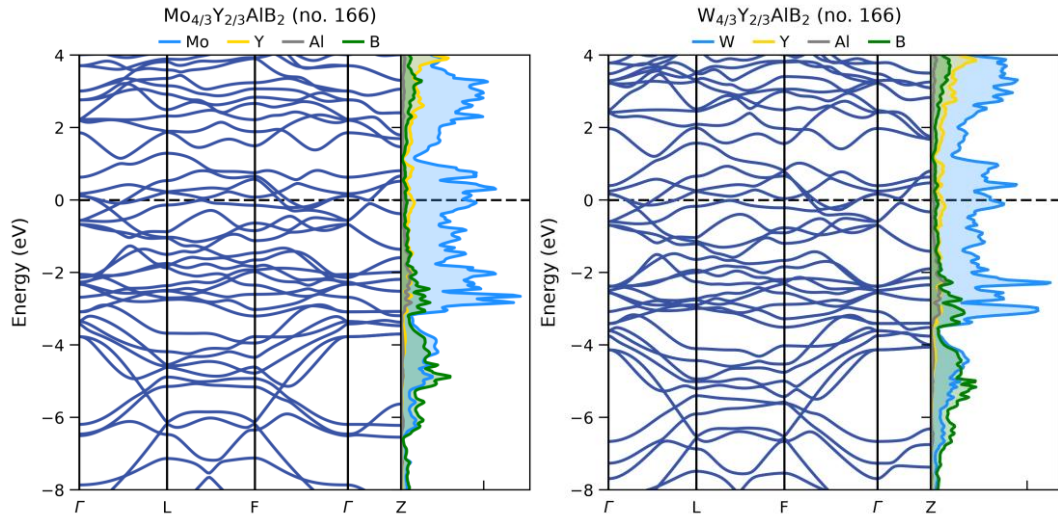


Figure S45. Calculated electronic band-structure and density of states for $\text{Mo}_{4/3}\text{Y}_{2/3}\text{AlB}_2$ and $\text{W}_{4/3}\text{Y}_{2/3}\text{AlB}_2$ *i*-MAB phases with $R\text{-}3m$ space group symmetry.

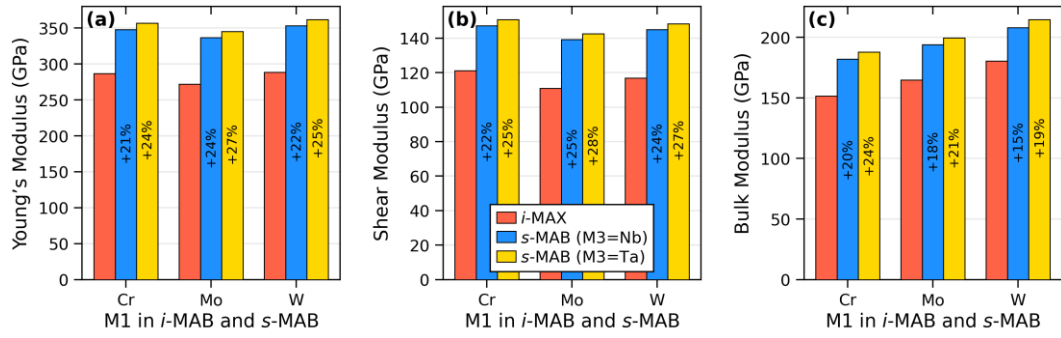


Figure S46. Comparison of (c) Young's, E , (d) shear, G , and (e) bulk, B , modulus for $\text{M1}_{4/3}\text{Y}_{2/3}\text{AlB}_2$ *i*-MAB in space group no. 166 and $\text{M1}_{4/3}\text{Y}_{2/3}\text{M3AlB}_4$ *s*-MAB in space group no. 191. Percentage change of *s*-MAB relative to *i*-MAB.