

Supporting Materials-III

Searching for Negative Thermal Expansion Materials with Bulk Framework Structures and their Relevant Scaling Relationships through Multi-step Machine Learning

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Table S1 Negative thermal expansion (NTE) prediction set (Oxides). T2 is the upper temperature limit, and the lower temperature limit is uniformly set as 0K. NTE is set to one decimal place, T2 to an integer.

No.	Formula	Crystal System	Probability (%)	NTE (ppm/K)	T2(K)
1	Ag ₂ (MoO ₄) ₃	orthorhombic	60%	-2.5	724
2	Ag ₂ IOF	monoclinic	80%	-21.5	263
3	Ag ₃ BO ₃	trigonal	60%	-5.0	256
4	Ag ₃ CN(ClO ₅) ₂	monoclinic	60%	-4.1	405
5	Ag ₃ Te(AsO ₇) ₂	monoclinic	60%	-4.5	349
6	Ag ₄ S(NO) ₂	orthorhombic	70%	-16.0	353
7	AgClO ₂	orthorhombic	60%	-12.9	213
8	AgClO ₃	cubic	60%	-9.2	247
9	AgCS(OF) ₃	trigonal	60%	-6.4	483
10	AgI ₃ N ₂ O	orthorhombic	60%	-18.0	402
11	AgSO ₃ F	monoclinic	90%	-4.3	314
12	Al ₁₁ (PO ₄) ₁₂	trigonal	80%	-11.4	582
13	Al ₂ Ga(PO ₄) ₃	monoclinic	60%	-6.7	528

14	$\text{Al}_2\text{P}_3\text{O}_{13}$	monoclinic	70%	-4.4	537
15	Al_2PO_8	orthorhombic	70%	-2.3	467
16	$\text{Al}_2\text{Se}_3\text{O}_{28}$	monoclinic	90%	-2.1	541
17	$\text{Al}_2\text{Si}_3(\text{NO}_5)_2$	orthorhombic	80%	-26.5	566
18	$\text{Al}_4\text{P}_5\text{HN}_2\text{O}_{21}$	monoclinic	60%	-7.9	491
19	AlAgO_2	orthorhombic	70%	-1.1	481
20	$\text{AlGa}(\text{PO}_4)_2$	monoclinic	70%	-5.4	431
21	AlSi_3O_8	monoclinic	70%	-4.2	486
22	$\text{AlSi}_5(\text{CO}_6)_2$	monoclinic	80%	-32.9	506
23	$\text{As}_2\text{W}_2\text{O}_{11}$	orthorhombic	60%	-6.6	637
24	AsO_2	orthorhombic	60%	-6.8	272
25	$\text{AsPHBr}_3\text{OF}_6$	orthorhombic	60%	-18.6	543
26	$\text{AsPHCl}_3\text{OF}_6$	orthorhombic	70%	-18.5	516
27	AsPO_4	orthorhombic	80%	-4.6	393
28	AsSClOF_8	monoclinic	60%	-6.9	537
29	AsWO_5	monoclinic	70%	-11.0	518
30	$\text{B}_4\text{N}_2\text{O}_{11}$ (Ferrimagnetic)	monoclinic	70%	-29.7	439
31	$\text{B}_4\text{N}_2\text{O}_{11}$ (Non-magnetic)	monoclinic	70%	-7.1	467
32	$\text{Ba}(\text{SO}_2)_4$	orthorhombic	70%	-5.0	1159
33	$\text{Ba}_2\text{SnSe}_4\text{O}_5$	orthorhombic	60%	-27.0	1161
34	BaBr_2O (Ferromagnetic)	orthorhombic	60%	-24.6	1186
35	BaBr_2O (Non-magnetic)	orthorhombic	60%	-24.5	1162
36	BaI_2O	orthorhombic	60%	-24.1	1165
37	$\text{BaMo}_2(\text{PO}_4)_3$	trigonal	80%	-0.7	1125
38	$\text{BaMo}_4\text{O}_{15}$	orthorhombic	70%	-1.0	1139
39	$\text{BaNb}_2\text{Fe}_2(\text{PO}_4)_6$	trigonal	70%	-2.3	1135
40	$\text{BaS}_2(\text{NO}_3)_2$	orthorhombic	60%	-7.4	1132
41	BaS_5O_8	orthorhombic	70%	-27.7	1246
42	$\text{BaSe}(\text{SO}_2)_4$	orthorhombic	60%	-23.8	1242
43	$\text{BaU}_2\text{P}_2\text{O}_{19}$	monoclinic	60%	-1.4	1053
44	$\text{BaU}_3\text{W}_3(\text{SeO}_7)_2$	orthorhombic	60%	-15.7	1030
45	$\text{Bi}(\text{PO}_3)_4$	orthorhombic	70%	-8.8	532
46	$\text{Bi}_2\text{P}_2\text{O}_9$	orthorhombic	70%	-6.7	508
47	Br_2O	orthorhombic	60%	-10.4	464
48	BrO_4	monoclinic	60%	-10.2	515
49	$\text{C}(\text{N}_2\text{O})_2$	orthorhombic	60%	-18.0	494
50	C_3O_2	orthorhombic	70%	-20.2	472

51	$C_4(N_3O)_3$	orthorhombic	60%	-17.3	504
52	$Ca(IO_6)_2$	orthorhombic	80%	-18.7	626
53	$Ca(Si_9O_{19})_2$	hexagonal	70%	-33.6	674
54	$Ca_2S_3(NO_6)_2$	cubic	70%	-6.6	638
55	Ca_2UO_{17}	orthorhombic	60%	-3.6	1098
56	$Ca_3W_2O_9$	orthorhombic	60%	-9.5	589
57	$CaC_2S_2(OF)_6$	trigonal	70%	-24.2	864
58	$CaFe_2Sb_2(PO_4)_6$	trigonal	60%	-2.6	720
59	$CaMo_2O_7$	monoclinic	60%	-5.5	644
60	$CaMo_2P_2O_9$	orthorhombic	90%	-2.1	638
61	$CaNiMoP_2O_9$	orthorhombic	70%	-1.1	655
62	CaP_4O_{11}	orthorhombic	60%	-5.9	693
63	$CaPNO_{11}$	monoclinic	80%	-4.8	642
64	CaW_2O_7	monoclinic	80%	-24.0	493
65	$Cd(NO_3)_2$	orthorhombic	80%	-6.8	357
66	Cd_2ClO_3	orthorhombic	70%	-16.2	391
67	$Cd_2Cu_2P_2SO_{17}$	orthorhombic	90%	-7.9	381
68	$Cd_2Ni(ClO_2)_6$	orthorhombic	80%	-9.6	481
69	$Cd_2Ni(ClO_2)_6$	orthorhombic	70%	-9.3	478
70	$Cd_2S_3(NO_6)_2$	cubic	80%	-6.3	651
71	$Cd_8S_2O_{23}$	monoclinic	80%	-4.8	612
72	CdC_3NO_6	orthorhombic	80%	-15.3	470
73	$CdCl_2O$	orthorhombic	60%	-12.1	439
74	$CdCN_3Cl_2O$	orthorhombic	60%	-14.5	443
75	$CdCo_3(PO_3)_8$	monoclinic	70%	-5.0	566
76	$CdCuP_2O_7$	monoclinic	90%	-3.8	210
77	$CdFe_2Sb_2(PO_4)_6$	trigonal	70%	-4.7	578
78	$CdFeC_5N_6O$	orthorhombic	80%	-17.7	669
79	$CdHC_2(NO)_4$	orthorhombic	80%	-29.0	570
80	$CdIClO_3$	orthorhombic	70%	-11.7	383
81	$CdPNO_5$	orthorhombic	80%	-8.2	334
82	$Ce(WO_4)_2$	cubic	100%	-17.1	1017
83	$CeMo_{12}(NO_{27})_2$	trigonal	70%	-5.6	1187
84	$CeMo_{12}(NO_{27})_2$	trigonal	70%	-5.6	1187
85	CN_6O	orthorhombic	60%	-18.0	487
86	CNO	orthorhombic	60%	-16.7	464
87	$Co_2Br_3(N_2O)_3$	monoclinic	60%	-12.6	407

88	$\text{Co}_2\text{Br}_3\text{N}_7\text{O}_2$	orthorhombic	60%	-13.4	405
89	$\text{Co}_2\text{CN}_9(\text{Cl}_2\text{O}_3)_2$	orthorhombic	70%	-19.5	604
90	$\text{Co}_3(\text{PO}_4)_4$	monoclinic	60%	-7.5	583
91	$\text{Co}_3\text{P}_4\text{O}_{15}$	orthorhombic	70%	-9.3	583
92	$\text{Co}_3\text{P}_6\text{WO}_{24}$	trigonal	90%	-8.4	679
93	$\text{Co}_4\text{Se}_3\text{Cl}_2\text{O}_9$	orthorhombic	60%	-7.6	381
94	$\text{Co}_6\text{Ge}_2(\text{CO})_{19}$	orthorhombic	80%	-3.6	669
95	CoAgO_2	hexagonal	70%	-0.4	401
96	$\text{CoAs}_3\text{OF}_{18}$	orthorhombic	60%	-6.0	707
97	$\text{CoCBrN}_4\text{O}_3$	orthorhombic	60%	-8.0	429
98	$\text{CoCuSe}_2(\text{ClO}_5)_2$	orthorhombic	80%	-7.2	492
99	CoN_7ClO_5	orthorhombic	60%	-20.0	457
100	CoNCl_4O_3	orthorhombic	70%	-15.2	490
101	CoO_2	orthorhombic	60%	-14.5	434
102	CoP_2O_7	monoclinic	60%	-9.0	445
103	$\text{CoP}_6(\text{WO}_8)_3$	trigonal	90%	-6.9	607
104	CoPNO_{10}	orthorhombic	80%	-5.3	546
105	CoPNO_5	orthorhombic	80%	-8.6	369
106	CoPO_4	orthorhombic	90%	-8.7	516
107	$\text{CoS}_2\text{N}_5\text{ClO}_4$	orthorhombic	60%	-18.2	476
108	CoSeO_3	monoclinic	60%	-1.9	650
109	CoSiO_4	orthorhombic	60%	-7.9	586
110	$\text{Cr}(\text{CO})_6$	orthorhombic	60%	-21.4	573
111	$\text{Cr}(\text{PO}_3)_4$	orthorhombic	90%	-1.3	753
112	$\text{Cr}_2(\text{PO}_4)_3$	trigonal	90%	-7.8	661
113	$\text{Cr}_2\text{Fe}_3\text{P}_6\text{WO}_{24}$	trigonal	90%	-3.5	605
114	$\text{Cr}_3(\text{CoO}_6)_2$	orthorhombic	70%	-2.7	755
115	$\text{Cr}_3(\text{CuO}_6)_2$	orthorhombic	70%	-1.8	747
116	$\text{Cr}_3(\text{FeO}_6)_2$	orthorhombic	70%	-2.8	787
117	$\text{Cr}_3(\text{PO}_4)_4$	monoclinic	90%	-13.7	687
118	$\text{Cr}_3\text{Co}(\text{PO}_4)_6$	trigonal	80%	-5.0	612
119	$\text{Cr}_3\text{Fe}(\text{PO}_4)_6$	trigonal	70%	-7.7	633
120	$\text{Cr}_3\text{Ni}(\text{PO}_4)_6$	trigonal	80%	-7.4	630
121	Cr_3O_7	orthorhombic	70%	-3.1	750
122	$\text{Cr}_3\text{P}_4\text{O}_{15}$	orthorhombic	90%	-10.3	689
123	$\text{Cr}_3\text{P}_6\text{WO}_{24}$	trigonal	100%	-8.3	681
124	$\text{Cr}_3\text{Sb}(\text{PO}_4)_6$	trigonal	80%	-4.4	641

125	$\text{Cr}_4(\text{PO}_4)_3$	orthorhombic	70%	-4.3	608
126	$\text{Cr}_4\text{CuO}_{12}$	monoclinic	60%	-0.7	559
127	Cr_5O_{12}	orthorhombic	70%	-3.9	684
128	CrC_5SO_7	orthorhombic	60%	-21.6	535
129	$\text{CrC}_6\text{N}_{12}(\text{ClO}_3)_3$	trigonal	60%	-19.5	763
130	$\text{CrFe}_3\text{Sb}_2(\text{PO}_4)_6$	trigonal	70%	-7.0	608
131	$\text{CrFe}_3\text{Sn}_2(\text{PO}_4)_6$	trigonal	70%	-7.0	608
132	CrN_3O_4	orthorhombic	90%	-17.3	598
133	$\text{CrN}_6(\text{ClO})_2$	orthorhombic	70%	-9.7	581
134	CrNiP_2O_9	orthorhombic	90%	-10.2	599
135	CrP_2O_7	monoclinic	80%	-10.1	633
136	$\text{CrP}_6(\text{WO}_8)_3$	trigonal	100%	-7.0	600
137	CrPO_4F	orthorhombic	90%	-9.9	657
138	CrWO_3	trigonal	60%	-15.1	547
139	$\text{CS}(\text{NO})_2$	orthorhombic	60%	-19.1	466
140	$\text{Cs}_3\text{CoI}_4\text{NO}_3$	orthorhombic	80%	-19.9	1295
141	$\text{CsC}(\text{OF})_2$	orthorhombic	60%	-2.9	1094
142	$\text{CsIn}_3\text{H}_6(\text{Se}_3\text{O}_{10})_2$	orthorhombic	60%	-1.6	1185
143	CsIOF_4	orthorhombic	60%	-15.6	1072
144	CsSbOF_4	orthorhombic	70%	-15.1	1181
145	$\text{Cu}(\text{NO}_3)_2$	orthorhombic	70%	-0.6	488
146	Cu_2NO_6	monoclinic	70%	-4.4	269
147	$\text{Cu}_2\text{P}_2\text{O}_7$	monoclinic	100%	-14.0	300
148	Cu_2SeO_4	cubic	80%	-3.0	418
149	$\text{Cu}_2\text{Te}_2\text{Pb}(\text{ClO}_3)_2$	monoclinic	60%	-10.7	256
150	$\text{Cu}_3\text{Mo}_2\text{O}_9$	orthorhombic	60%	-2.0	712
151	Cu_3OF_5	monoclinic	60%	-5.4	239
152	$\text{Cu}_3\text{P}_2\text{NO}_6$	orthorhombic	80%	-14.0	397
153	Cu_3SeO_8	orthorhombic	60%	-4.6	333
154	$\text{Cu}_5\text{SeCl}_5\text{O}_4$	monoclinic	60%	-13.5	357
155	CuCClO	orthorhombic	60%	-13.3	290
156	CuClO_2	monoclinic	70%	-14.1	319
157	CuCO_3	monoclinic	80%	-3.7	439
158	$\text{CuHS}(\text{NO})_4$	orthorhombic	70%	-31.1	496
159	$\text{CuMo}_3\text{O}_{11}$	orthorhombic	60%	-5.6	622
160	CuO	orthorhombic	60%	-2.4	412
161	CuPO_4	orthorhombic	90%	-7.7	407

162	CuSeClO ₅	orthorhombic	70%	-6.8	455
163	CuSiO ₄	trigonal	60%	-1.6	563
164	CuSN ₄ O ₅	orthorhombic	80%	-17.5	431
165	Dy ₂ (MoO ₄) ₃	orthorhombic	100%	-18.7	1183
166	Dy ₂ (SeO ₄) ₃	orthorhombic	100%	-8.7	1067
167	Dy ₂ Mo ₈ O ₃₃	monoclinic	80%	-7.8	1116
168	DyRe ₃ O ₁₆	orthorhombic	100%	-14.1	1089
169	DySeClO ₃	orthorhombic	90%	-10.2	995
170	ErSeClO ₃	orthorhombic	90%	-10.2	995
171	Eu ₂ (MoO ₄) ₃	orthorhombic	70%	-18.3	1175
172	Eu ₂ Mo ₅ O ₁₈	orthorhombic	90%	-13.5	1110
173	Eu ₄ Br ₆ O	hexagonal	70%	-15.3	1138
174	EuBr ₂ O	orthorhombic	60%	-13.5	1138
175	EuSeClO ₃	orthorhombic	90%	-9.0	1020
176	EuTl(MoO ₄) ₂	orthorhombic	60%	-14.5	1020
177	Fe(Bi ₅ O ₈) ₅	monoclinic	60%	-8.3	668
178	Fe(PO ₃) ₄	monoclinic	60%	-7.7	667
179	Fe ₂ Cu(PO ₅) ₂	monoclinic	100%	-13.0	465
180	Fe ₂ P ₃ O ₁₃	monoclinic	90%	-7.5	636
181	Fe ₂ Sb(PO ₄) ₃	trigonal	60%	-7.1	603
182	Fe ₂ Sn(PO ₄) ₃	trigonal	60%	-3.6	602
183	Fe ₃ (P ₂ O ₇) ₂	orthorhombic	80%	-10.4	690
184	Fe ₃ (PO ₄) ₄	monoclinic	90%	-10.1	663
185	Fe ₃ Co ₂ P ₆ WO ₂₄	trigonal	70%	-6.1	584
186	Fe ₃ Co ₂ Sb(PO ₄) ₆	trigonal	60%	-6.4	602
187	Fe ₃ CoSb ₂ (PO ₄) ₆	trigonal	60%	-7.1	589
188	Fe ₃ Cu ₂ Sb(PO ₄) ₆	trigonal	90%	-2.8	593
189	Fe ₃ Cu ₂ Sn(PO ₄) ₆	trigonal	90%	-2.8	598
190	Fe ₃ Ni ₂ P ₆ WO ₂₄	trigonal	70%	-4.2	595
191	Fe ₃ Ni ₂ Sn(PO ₄) ₆	trigonal	60%	-4.2	552
192	Fe ₃ NiSb ₂ (PO ₄) ₆	trigonal	60%	-3.5	591
193	Fe ₃ NiSn ₂ (PO ₄) ₆	trigonal	60%	-3.5	591
194	Fe ₃ P ₄ O ₁₅	orthorhombic	80%	-10.5	664
195	Fe ₃ P ₆ WO ₂₄	trigonal	90%	-8.6	676
196	Fe ₃ Sb(PO ₄) ₆	trigonal	70%	-5.5	638
197	Fe ₄ Te ₂ MoC ₁₄ (SO ₇) ₂	orthorhombic	70%	-7.7	957
198	Fe ₅ P ₆ WO ₂₄	trigonal	70%	-6.1	591

199	$\text{Fe}_7\text{Sb}_3\text{P}_3(\text{ClO}_6)_3$	orthorhombic	60%	-6.8	575
200	$\text{FeAs}_2\text{H}_3\text{OF}_{13}$	orthorhombic	60%	-11.8	725
201	FeBiO_3	trigonal	60%	-12.1	502
202	$\text{FeC}_3\text{NCl}_3\text{O}_2$	orthorhombic	60%	-21.6	638
203	$\text{FeC}_4\text{N}_2\text{O}_9$	monoclinic	70%	-7.6	568
204	$\text{FeCu}_2\text{As}_3\text{O}_{11}$	orthorhombic	60%	-9.0	617
205	$\text{FeH}_2\text{Cl}_5\text{O}_3$	orthorhombic	60%	-26.0	651
206	$\text{FeN}_2\text{Cl}_5\text{O}$	orthorhombic	60%	-17.2	526
207	$\text{FeNi}_3\text{Sn}_2(\text{PO}_4)_6$	trigonal	60%	-6.2	555
208	FeNiP_2O_9	orthorhombic	80%	-10.3	615
209	FeP_2O_7	monoclinic	70%	-10.5	575
210	$\text{FeP}_6(\text{WO}_8)_3$	trigonal	90%	-7.0	607
211	$\text{FePbC}_5\text{N}_6\text{O}$	orthorhombic	70%	-14.4	645
212	FePO_4	orthorhombic	100%	-8.8	563
213	$\text{FeSb}(\text{P}_2\text{O}_7)_2$	orthorhombic	80%	-1.7	740
214	$\text{FeSiP}_3\text{O}_{11}$	trigonal	60%	-4.1	673
215	$\text{Ga}_2(\text{WO}_4)_3$	orthorhombic	100%	-12.2	1011
216	$\text{Ga}_2\text{Fe}(\text{PO}_4)_3$	monoclinic	100%	-9.1	666
217	$\text{Ga}_4\text{SbS}_9\text{N}_3\text{O}_2$	cubic	70%	-14.8	672
218	GaO	hexagonal	60%	-6.1	318
219	GaP_2O_9	monoclinic	80%	-5.2	568
220	$\text{Gd}(\text{ReO}_5)_3$	orthorhombic	100%	-13.2	1083
221	$\text{Gd}_2(\text{MoO}_4)_3$	orthorhombic	90%	-17.9	1177
222	$\text{Gd}_2(\text{WO}_4)_3$	orthorhombic	100%	-19.7	1127
223	$\text{Gd}_2\text{Mo}_5\text{O}_{18}$	orthorhombic	90%	-13.5	1112
224	$\text{Gd}_3(\text{BrO}_3)_2$	orthorhombic	60%	-14.1	985
225	GdSeClO_3	orthorhombic	80%	-9.2	998
226	$\text{Ge}_2\text{RuC}_4(\text{Cl}_3\text{O}_2)_2$	monoclinic	70%	-16.4	659
227	GePClO_2	orthorhombic	70%	-11.5	393
228	GeWO_4	cubic	80%	-16.8	471
229	$\text{H}_2\text{Os}_5(\text{CO})_{16}$	orthorhombic	60%	-7.0	580
230	$\text{Hf}(\text{PO}_5)_2$	monoclinic	70%	-6.3	644
231	$\text{Hf}_2\text{P}_2\text{O}_9$	orthorhombic	70%	-3.6	607
232	HfP_2O_7	cubic	90%	-11.1	514
233	HgNO_3	monoclinic	60%	-7.4	395
234	$\text{Ho}_2(\text{SeO}_4)_3$	orthorhombic	100%	-9.0	1065
235	$\text{Ho}_2(\text{SO}_4)_3$	trigonal	70%	-6.2	1081

236	HoH ₁₆ C ₂ S ₂ NO ₁₂	orthorhombic	60%	-1.2	1085
237	HoSeClO ₃	orthorhombic	90%	-10.2	996
238	HoTeClO ₃	orthorhombic	60%	-15.4	973
239	HRuN ₆ Cl ₃ O	orthorhombic	60%	-23.2	493
240	HS ₂ N(O ₂ F) ₂	monoclinic	60%	-16.8	388
241	InPO ₄	orthorhombic	60%	-0.4	315
242	K ₂ InBr ₅ O	orthorhombic	70%	-22.9	1221
243	K ₂ RuI ₅ NO	orthorhombic	60%	-20.8	1245
244	K ₃ Mo ₁₂ PO ₄₀	cubic	70%	-0.6	1205
245	K ₃ P(W ₃ O ₁₀) ₄	cubic	80%	-1.0	1108
246	K ₃ TaO ₂ F ₇ (Pnma)	orthorhombic	60%	-19.3	1070
247	K ₃ TaO ₂ F ₇ (Pna2_1)	orthorhombic	60%	-19.3	1066
248	K ₄ H ₄ WC ₈ (N ₄ O) ₂	orthorhombic	60%	-24.9	1165
249	K Al (SO ₇) ₂	cubic	90%	-27.8	1334
250	KMo ₂ (PO ₄) ₃	orthorhombic	100%	-5.7	1191
251	KNiPO ₁₀	monoclinic	80%	-3.1	1100
252	KP(OF) ₂	orthorhombic	70%	-0.1	1092
253	KTb(N ₂ O ₇) ₂	orthorhombic	60%	-4.0	1067
254	KU ₂ (PO ₄) ₃	trigonal	90%	-5.6	1035
255	KVOF ₃	orthorhombic	60%	-14.6	1096
256	KZr ₂ (AsO ₄) ₃	trigonal	60%	-2.7	1124
257	La ₂ Te ₃ MoO ₁₂	orthorhombic	70%	-0.3	1041
258	La ₂ TeMo ₆ O ₃₅	monoclinic	90%	-4.5	1210
259	Li ₂ CoSn ₃ (PO ₄) ₆	trigonal	90%	-2.6	681
260	Li ₂ Fe ₂ (WO ₄) ₃	orthorhombic	60%	-3.7	770
261	Li ₂ MnSi ₃ O ₈	monoclinic	60%	-1.5	464
262	Li ₂ NiSn ₃ (PO ₄) ₆	trigonal	80%	-0.4	691
263	Li ₂ Pd(N ₂ O ₅) ₂	orthorhombic	60%	-9.1	599
264	Li ₂ Sn ₂ (SO ₄) ₃	orthorhombic	70%	-4.5	664
265	Li ₂ TiSn ₃ (PO ₄) ₆	trigonal	80%	-2.3	752
266	Li ₂ V ₂ Sn(PO ₄) ₃	monoclinic	70%	-1.1	554
267	Li ₃ In ₂ (PO ₄) ₃	trigonal	80%	-0.2	543
268	Li ₃ Sb ₂ (PO ₄) ₃	trigonal	90%	-5.5	531
269	Li ₃ Sn ₂ (PO ₄) ₃	trigonal	90%	-6.1	534
270	Li ₄ V ₃ P ₈ O ₂₉	monoclinic	60%	-2.2	712
271	LiAl(PO ₃) ₄	orthorhombic	70%	-4.2	617
272	LiAlGeO ₄	trigonal	80%	-1.1	467

273	LiAlS ₃ (Cl ₂ O ₃) ₂	orthorhombic	70%	-24.0	688
274	LiBi(PO ₃) ₄	orthorhombic	70%	-6.9	664
275	LiCo(PO ₃) ₄	orthorhombic	80%	-8.6	635
276	LiCo ₂ (CO ₃) ₄	monoclinic	70%	-6.5	560
277	LiCo ₂ (PO ₄) ₃	monoclinic	70%	-3.1	708
278	LiCo ₃ Sb(PO ₄) ₆	trigonal	90%	-6.5	671
279	LiCoSiO ₄	monoclinic	60%	-4.5	562
280	LiCr(PO ₃) ₄	orthorhombic	70%	-6.4	637
281	LiCr ₄ (PO ₄) ₃	orthorhombic	60%	-2.1	689
282	LiCu(PO ₃) ₃	orthorhombic	70%	-3.4	679
283	LiFe(PO ₃) ₄	orthorhombic	70%	-8.0	639
284	LiFe ₂ (CO ₃) ₄	monoclinic	60%	-8.4	568
285	LiFe ₂ OF ₃	orthorhombic	60%	-11.3	547
286	LiFe ₆ (OF ₂) ₄	monoclinic	70%	-3.4	475
287	LiGa(PO ₃) ₄	orthorhombic	80%	-7.5	646
288	LiGePCO ₇	monoclinic	60%	-1.1	586
289	LiHfPCO ₇	monoclinic	60%	-4.1	621
290	LiInP ₂ O ₇	monoclinic	60%	-1.5	653
291	LiMn(PO ₃) ₃	orthorhombic	60%	-7.3	673
292	LiMn(PO ₃) ₄	orthorhombic	80%	-8.5	636
293	LiMn ₄ (PO ₄) ₃	orthorhombic	60%	-7.9	508
294	LiMo(PO ₃) ₄	orthorhombic	80%	-10.1	703
295	LiMo ₂ (PO ₄) ₃	monoclinic	70%	-6.4	650
296	LiMo ₂ P ₂ O ₉	orthorhombic	70%	-2.9	719
297	LiMo ₂ P ₃ O ₁₃	monoclinic	70%	-9.0	626
298	LiNb(PO ₃) ₄	orthorhombic	70%	-8.5	688
299	LiNbCo ₃ (PO ₄) ₆	trigonal	80%	-5.3	723
300	LiNbSn ₃ (PO ₄) ₆	trigonal	80%	-3.4	734
301	LiNi(PO ₃) ₃	orthorhombic	70%	-4.1	667
302	LiNi(PO ₃) ₄	orthorhombic	80%	-8.4	630
303	LiNi ₂ OF ₃	orthorhombic	70%	-11.3	534
304	LiNi ₂ P ₃ O ₁₁	monoclinic	60%	-7.0	591
305	LiNiP ₂ O ₇	monoclinic	60%	-1.6	586
306	LiP(WO ₄) ₂	monoclinic	60%	-6.8	544
307	LiP ₃ (WO ₆) ₂	monoclinic	80%	-2.4	648
308	LiP ₃ W ₂ O ₁₃	monoclinic	80%	-8.9	534
309	LiP ₄ WO ₁₂	orthorhombic	90%	-11.1	681

310	LiPWCO ₇	monoclinic	60%	-7.9	588
311	LiS ₂ N ₃ O ₈	monoclinic	70%	-8.5	554
312	LiSb(PO ₃) ₄	monoclinic	60%	-4.8	644
313	LiSbP ₂ O ₇	orthorhombic	60%	-2.2	703
314	LiSn(PO ₃) ₃	orthorhombic	80%	-6.7	668
315	LiSn(PO ₃) ₄	orthorhombic	80%	-10.0	657
316	LiSn ₂ (PO ₄) ₃	orthorhombic	70%	-4.5	645
317	LiSn ₄ (PO ₄) ₃	orthorhombic	60%	-3.4	569
318	LiTi(PO ₃) ₄	orthorhombic	70%	-4.4	672
319	LiTi ₂ P ₃ O ₁₁	monoclinic	60%	-5.1	627
320	LiTi ₃ Nb(PO ₄) ₆	trigonal	70%	-3.9	696
321	LiTi ₃ Sb(PO ₄) ₆	trigonal	80%	-6.2	709
322	LiTi ₃ V(PO ₄) ₆	trigonal	70%	-4.9	686
323	LiV(PO ₃) ₃	orthorhombic	60%	-7.5	694
324	LiV(PO ₃) ₄	orthorhombic	70%	-4.8	657
325	LiV ₂ P ₃ O ₁₁	monoclinic	60%	-6.5	591
326	LiVCo ₃ (PO ₄) ₆	trigonal	80%	-1.8	706
327	LiVSn ₃ (PO ₄) ₆	trigonal	80%	-3.6	692
328	LiZr ₂ (AsO ₄) ₃	trigonal	70%	-0.4	660
329	LiZr ₂ (PO ₄) ₃	monoclinic	80%	-2.3	745
330	Lu(PO ₃) ₃	trigonal	80%	-7.6	1126
331	LuSeClO ₃	orthorhombic	80%	-9.4	938
332	Mg ₂ Tl ₂ (MoO ₄) ₃	cubic	80%	-9.1	826
333	MgBr ₂ O	orthorhombic	60%	-27.4	492
334	MgCd ₂ (ClO ₂) ₆ (Total Magnetization= 8.00 μB/f.u.)	orthorhombic	80%	-26.5	552
335	MgCd ₂ (ClO ₂) ₆ (Total Magnetization= 4.00 μB/f.u.)	orthorhombic	80%	-21.2	543
336	MgH ₆ S ₂ O ₃	orthorhombic	60%	-30.0	580
337	MgMo ₂ O ₇	monoclinic	80%	-5.0	655
338	MgMo ₂ P ₂ O ₉	orthorhombic	90%	-6.1	545
339	MgP ₂ W ₂ O ₉	orthorhombic	70%	-7.5	519
340	MgS ₈ (O ₅ F ₂) ₄	monoclinic	70%	-26.6	592
341	MgTe(BrO) ₆	cubic	80%	-23.5	698
342	MgTe(ClO) ₆	trigonal	70%	-24.0	435
343	MgTe(IO) ₆	cubic	80%	-25.3	676
344	MgU ₂ Cr ₂ O ₁₆	orthorhombic	80%	-2.6	1078
345	MgVFeMo ₃ O ₁₄	monoclinic	60%	-3.9	616

346	MgW ₂ O ₇	monoclinic	70%	-6.3	593
347	Mn(C ₂ O ₃) ₂	trigonal	70%	-18.4	372
348	Mn ₂ Al ₃ Fe(PO ₇) ₃	monoclinic	70%	-8.6	521
349	Mn ₂ Cr ₃ (NO ₆) ₂	cubic	60%	-9.0	864
350	Mn ₂ Cr ₃ O ₁₂	orthorhombic	70%	-3.6	731
351	Mn ₂ CrFe ₃ (PO ₄) ₆	trigonal	70%	-2.0	641
352	Mn ₂ CrNi ₃ (PO ₄) ₆	trigonal	70%	-6.5	569
353	Mn ₂ Cu(PO ₄) ₃	trigonal	80%	-0.5	447
354	Mn ₂ Fe ₃ Cu(PO ₄) ₆	trigonal	70%	-5.8	567
355	Mn ₂ Fe ₃ Ni(PO ₄) ₆	trigonal	60%	-5.8	558
356	Mn ₂ Fe ₃ P ₆ WO ₂₄	trigonal	70%	-3.8	583
357	Mn ₂ Fe ₃ Sb(PO ₄) ₆	trigonal	60%	-3.9	571
358	Mn ₂ Fe ₃ Sn(PO ₄) ₆	trigonal	60%	-3.7	603
359	Mn ₂ NbFe ₃ (PO ₄) ₆	trigonal	70%	-2.4	695
360	Mn ₂ NbNi ₃ (PO ₄) ₆	trigonal	70%	-4.0	637
361	Mn ₂ NbV ₃ (PO ₄) ₆	trigonal	70%	-0.5	687
362	Mn ₂ Ni ₃ P ₆ WO ₂₄	trigonal	70%	-7.5	598
363	Mn ₂ P ₂ O ₇ F ₂	orthorhombic	70%	-6.3	550
364	Mn ₂ P ₂ O ₉	orthorhombic	70%	-7.3	520
365	Mn ₂ Tl ₂ (MoO ₄) ₃	cubic	70%	-16.0	921
366	Mn ₂ Tl ₂ (SO ₄) ₃	cubic	60%	-2.8	626
367	Mn ₂ V ₃ Cr(PO ₄) ₆	trigonal	70%	-0.6	640
368	Mn ₂ V ₃ Cu(PO ₄) ₆	trigonal	70%	-0.7	647
369	Mn ₂ V ₃ P ₆ WO ₂₄	trigonal	70%	-3.7	583
370	Mn ₂ V ₃ Sb(PO ₄) ₆	trigonal	60%	-2.3	659
371	Mn ₂ V ₃ Sn(PO ₄) ₆	trigonal	60%	-1.6	682
372	Mn ₂ VF ₃ (PO ₄) ₆	trigonal	60%	-1.5	653
373	Mn ₂ VNi ₃ (PO ₄) ₆	trigonal	60%	-6.9	583
374	Mn ₃ (P ₂ O ₇) ₂	orthorhombic	90%	-6.2	590
375	Mn ₃ (PO ₄) ₄	monoclinic	70%	-9.5	566
376	Mn ₃ (PO ₇) ₂	monoclinic	70%	-9.8	523
377	Mn ₃ Cr(PO ₄) ₆	trigonal	90%	-7.9	617
378	Mn ₃ Cr ₂ Sb(PO ₄) ₆	trigonal	90%	-4.2	583
379	Mn ₃ Cr ₂ Sn(PO ₄) ₆	trigonal	90%	-4.0	636
380	Mn ₃ CrSn ₂ (PO ₄) ₆	trigonal	70%	-7.0	592
381	Mn ₃ CrTe ₂ (PO ₄) ₆	trigonal	60%	-3.8	601
382	Mn ₃ Cu ₂ Sn(PO ₄) ₆	trigonal	80%	-2.8	416

383	$\text{Mn}_3\text{Fe}_2\text{P}_6\text{WO}_{24}$	trigonal	70%	-7.5	588
384	$\text{Mn}_3\text{Fe}_2\text{Sb}(\text{PO}_4)_6$	trigonal	60%	-7.3	576
385	$\text{Mn}_3\text{Fe}_2\text{Sn}(\text{PO}_4)_6$	trigonal	60%	-6.4	631
386	$\text{Mn}_3\text{FeSn}_2(\text{PO}_4)_6$	trigonal	60%	-7.1	591
387	$\text{Mn}_3\text{Nb}(\text{PO}_4)_6$	trigonal	90%	-8.1	698
388	$\text{Mn}_3\text{NbCo}_2(\text{PO}_4)_6$	trigonal	70%	-4.5	630
389	$\text{Mn}_3\text{NbCr}_2(\text{PO}_4)_6$	trigonal	90%	-3.8	622
390	$\text{Mn}_3\text{NbFe}_2(\text{PO}_4)_6$	trigonal	70%	-5.2	620
391	$\text{Mn}_3\text{NbNi}_2(\text{PO}_4)_6$	trigonal	70%	-4.9	621
392	$\text{Mn}_3\text{Ni}_2\text{P}_6\text{WO}_{24}$	trigonal	70%	-6.6	582
393	Mn_3O_4	monoclinic	70%	-16.3	485
394	$\text{Mn}_3\text{P}_6\text{WO}_{24}$	trigonal	90%	-8.5	665
395	$\text{Mn}_3\text{Sb}(\text{PO}_4)_6$	trigonal	60%	-4.6	535
396	$\text{Mn}_3\text{Sn}(\text{PO}_4)_6$	trigonal	60%	-3.0	538
397	$\text{Mn}_3\text{V}(\text{PO}_4)_6$	trigonal	70%	-8.2	640
398	$\text{Mn}_3\text{VCr}_2(\text{PO}_4)_6$	trigonal	90%	-1.3	614
399	$\text{Mn}_3\text{VCu}_2(\text{PO}_4)_6$	trigonal	90%	-2.4	637
400	$\text{Mn}_3\text{VFe}_2(\text{PO}_4)_6$	trigonal	60%	-4.4	577
401	$\text{Mn}_3\text{VSb}_2(\text{PO}_4)_6$	trigonal	70%	-4.6	671
402	$\text{Mn}_3\text{VTe}_2(\text{PO}_4)_6$	trigonal	60%	-4.3	683
403	$\text{Mn}_5\text{Cu}(\text{PO}_4)_4$	monoclinic	70%	-2.2	422
404	$\text{Mn}_5\text{Cu}(\text{PO}_4)_6$	trigonal	60%	-0.2	451
405	$\text{Mn}_5\text{P}_6\text{WO}_{24}$	trigonal	80%	-2.7	642
406	MnAsNO_5	orthorhombic	70%	-7.0	409
407	MnAsO_5	monoclinic	60%	-5.9	359
408	MnC_3BrO_5	orthorhombic	60%	-15.2	463
409	$\text{MnC}_6\text{S}_2\text{NO}_5\text{F}_6$	orthorhombic	60%	-7.1	618
410	$\text{MnCr}_3(\text{PO}_4)_6$	trigonal	90%	-8.0	616
411	$\text{MnFe}(\text{PO}_4)_2$	trigonal	60%	-1.1	630
412	$\text{MnFe}_2(\text{PO}_4)_3$	trigonal	60%	-5.8	554
413	$\text{MnFe}_2\text{Sb}_2(\text{PO}_4)_6$	trigonal	60%	-5.5	665
414	$\text{MnFe}_3\text{Sb}_2(\text{PO}_4)_6$	trigonal	60%	-7.5	602
415	$\text{MnFe}_3\text{Sn}_2(\text{PO}_4)_6$	trigonal	60%	-6.6	593
416	$\text{MnH}_{12}\text{C}_2\text{NCl}_3\text{O}_2$	orthorhombic	60%	-25.5	593
417	$\text{MnNb}_3(\text{PO}_4)_6$	trigonal	90%	-8.3	695
418	MnNO_4	orthorhombic	80%	-19.1	443
419	MnO_2	orthorhombic	60%	-16.8	501

420	MnP ₂ O ₇	cubic	70%	-8.7	469
421	MnP ₆ (WO ₈) ₃	trigonal	100%	-7.4	583
422	MnPCO ₄	orthorhombic	60%	-22.0	470
423	MnPNO ₅	orthorhombic	90%	-10.6	381
424	MnPO ₄	orthorhombic	80%	-8.2	452
425	MnRe(CO) ₁₀	monoclinic	70%	-11.4	468
426	MnSeO ₄	orthorhombic	70%	-6.4	329
427	MnSO ₆	orthorhombic	80%	-8.4	484
428	MnTeC ₅ O ₆ F ₅	orthorhombic	70%	-12.2	471
429	MnTl(PO ₃) ₃	orthorhombic	60%	-7.8	468
430	MnV ₂ (PO ₄) ₃	trigonal	60%	-0.4	648
431	MnV ₂ O ₈	orthorhombic	60%	-5.9	617
432	MnV ₃ (PO ₄) ₆	trigonal	70%	-8.2	634
433	MnV ₃ Co ₂ (PO ₄) ₆	trigonal	60%	-4.9	559
434	MnV ₃ Cu ₂ (PO ₄) ₆	trigonal	90%	-1.2	649
435	MnV ₃ Ni ₂ (PO ₄) ₆	trigonal	60%	-5.9	560
436	MnV ₅ (PO ₄) ₆	trigonal	60%	-4.0	584
437	Mo(CO) ₆	orthorhombic	60%	-22.8	593
438	Mo(PO ₃) ₄	orthorhombic	90%	-8.2	744
439	Mo ₂ (PO ₄) ₃	monoclinic	80%	-8.5	722
440	Mo ₂ C ₅ N ₃ O ₁₄	orthorhombic	90%	-20.3	611
441	Mo ₂ P ₂ O ₁₁	orthorhombic	100%	-10.7	756
442	Mo ₂ P ₂ O ₉	orthorhombic	100%	-10.5	681
443	Mo ₂ P ₃ O ₁₁	monoclinic	90%	-10.8	765
444	Mo ₂ P ₃ O ₁₃	monoclinic	100%	-9.8	719
445	Mo ₂ P ₄ O ₁₅	monoclinic	100%	-9.4	729
446	Mo ₂ PO ₈	monoclinic	80%	-10.4	637
447	Mo ₃ (NO ₅) ₂	orthorhombic	80%	-9.2	639
448	Mo ₃ (PO ₄) ₄	monoclinic	90%	-10.7	764
449	Mo ₃ O ₇	orthorhombic	90%	-10.1	722
450	Mo ₃ P ₅ Pb ₃ O ₂₃	orthorhombic	60%	-9.2	617
451	Mo ₃ PW ₉ N ₃ O ₄₀	orthorhombic	80%	-15.7	803
452	Mo ₄ O ₁₁	orthorhombic	70%	-10.4	671
453	MoCl ₂ O ₃	orthorhombic	70%	-16.7	644
454	MoN ₂ Cl ₅ O	orthorhombic	60%	-19.9	572
455	MoO ₃	hexagonal	70%	-7.9	628
456	MoP ₂ O ₇	cubic	100%	-10.3	662

457	MoPCl ₈ O	orthorhombic	80%	-17.3	606
458	MoPO ₅	orthorhombic	100%	-10.8	603
459	MoRhN ₅ ClO ₄	orthorhombic	60%	-22.3	653
460	MoSO ₆	orthorhombic	60%	-0.3	813
461	N ₂ O	cubic	60%	-17.6	366
462	N ₂ O ₃ (Ferrimagnetic)	orthorhombic	70%	-13.3	373
463	N ₂ O ₃ (Antiferromagnetic)	orthorhombic	70%	-6.6	370
464	N ₄ O ₉	monoclinic	70%	-4.7	485
465	Na ₂ FeSn(PO ₄) ₃	monoclinic	80%	-3.1	702
466	Na ₂ OsO ₇	monoclinic	60%	-7.3	644
467	Na ₂ OsO ₈	monoclinic	60%	-2.7	632
468	Na ₂ Pr ₄ Br ₉ NO	monoclinic	70%	-18.8	1154
469	Na ₃ Be ₃ B ₃ P ₆ O ₂₅	cubic	70%	-0.2	672
470	Na ₈ Al ₆ Si ₆ CO ₂₇	trigonal	70%	-2.7	578
471	Na ₈ Al ₆ Si ₆ O ₂₅ (Band gap=4.30)	trigonal	70%	-3.5	496
472	Na ₈ Al ₆ Si ₆ O ₂₅ (Band gap=1.87)	trigonal	70%	-3.5	492
473	NaAlSiO ₄	cubic	60%	-3.9	502
474	NaB ₆ S ₄ (I ₃ O ₄) ₂	orthorhombic	70%	-21.9	860
475	NaBrO ₃	cubic	80%	-24.3	684
476	NaClO ₃	cubic	70%	-2.4	677
477	NaGePCO ₇	monoclinic	60%	-1.2	683
478	NaHfPCO ₇	monoclinic	60%	-3.6	658
479	NaMg(PO ₃) ₃	cubic	90%	-0.7	688
480	NaMn ₂ FeAg(PO ₄) ₃	monoclinic	60%	-3.2	642
481	NaMnH ₃ (CO ₂) ₃	cubic	60%	-22.1	941
482	NaMo ₂ (PO ₄) ₃	trigonal	80%	-4.8	596
483	NaMo ₂ P ₂ O ₉	orthorhombic	70%	-2.2	670
484	NaMo ₃ NO ₁₀	orthorhombic	70%	-6.2	579
485	NaMo ₃ O ₁₁	orthorhombic	70%	-4.2	579
486	NaNb ₄ (PO ₄) ₆	trigonal	80%	-2.3	795
487	NaNi ₄ (P ₂ O ₁₁) ₂	monoclinic	90%	-8.6	646
488	NaSbPCO ₇	monoclinic	60%	-3.2	691
489	NaSn ₂ (PO ₄) ₃	trigonal	80%	-2.8	688
490	NaTi ₂ O ₄	orthorhombic	60%	-33.1	613
491	NaW ₂ (Br ₃ O) ₂	orthorhombic	60%	-17.9	594
492	NaZn(PO ₃) ₃	cubic	80%	-1.2	726
493	NaZr ₂ (AsO ₄) ₃	trigonal	70%	-3.0	683

494	$\text{NaZr}_2(\text{PO}_4)_3$	trigonal	100%	-0.2	756
495	$\text{Nb}(\text{Br}_3\text{O})_2$	orthorhombic	60%	-9.7	712
496	$\text{Nb}(\text{PO}_3)_4$	orthorhombic	90%	-8.8	739
497	$\text{Nb}_{12}\text{WO}_{33}$	monoclinic	90%	-4.4	688
498	$\text{Nb}_2(\text{PO}_4)_3$	trigonal	90%	-8.3	783
499	$\text{Nb}_2\text{Ge}_2\text{O}_7$	monoclinic	70%	-0.1	656
500	$\text{Nb}_2\text{P}_2\text{O}_9$	orthorhombic	90%	-9.7	661
501	$\text{Nb}_2\text{S}_4\text{Cl}_9\text{O}_5$	orthorhombic	70%	-15.1	617
502	$\text{Nb}_3(\text{Cl}_3\text{O}_4)_2$	cubic	80%	-8.5	727
503	$\text{Nb}_3(\text{OF})_5$	orthorhombic	70%	-11.2	635
504	$\text{Nb}_3\text{Al}(\text{PO}_4)_6$	trigonal	90%	-7.5	691
505	Nb_3ClO_7	orthorhombic	70%	-6.4	594
506	$\text{Nb}_3\text{Co}(\text{PO}_4)_6$	trigonal	80%	-8.0	696
507	$\text{Nb}_3\text{Cr}(\text{PO}_4)_6$	trigonal	90%	-8.8	724
508	$\text{Nb}_3\text{Fe}(\text{PO}_4)_6$	trigonal	80%	-8.1	697
509	$\text{Nb}_3\text{Ni}(\text{PO}_4)_6$	trigonal	80%	-7.7	696
510	$\text{Nb}_3\text{O}_7\text{F}$	orthorhombic	70%	-7.1	580
511	$\text{Nb}_3\text{P}_6\text{WO}_{24}$	trigonal	100%	-8.1	711
512	$\text{Nb}_3\text{Sb}(\text{PO}_4)_6$	trigonal	90%	-7.9	731
513	$\text{Nb}_3\text{V}(\text{PO}_4)_6$	trigonal	90%	-8.2	721
514	$\text{Nb}_8\text{P}_{15}\text{O}_{56}$	trigonal	100%	-4.4	802
515	$\text{Nb}_9\text{AsO}_{25}$	monoclinic	70%	-3.3	591
516	$\text{Nb}_9\text{PO}_{25}$	monoclinic	60%	-5.4	590
517	$\text{NbCr}_2\text{Fe}_3(\text{PO}_4)_6$	trigonal	90%	-3.1	691
518	$\text{NbCr}_3(\text{PO}_4)_6$	trigonal	90%	-8.6	730
519	$\text{NbFe}_3(\text{PO}_4)_6$	trigonal	80%	-8.2	697
520	$\text{NbFe}_3\text{Co}_2(\text{PO}_4)_6$	trigonal	70%	-6.3	611
521	$\text{NbFe}_3\text{Cu}_2(\text{PO}_4)_6$	trigonal	90%	-4.2	626
522	$\text{NbFe}_5(\text{PO}_4)_6$	trigonal	70%	-6.2	618
523	NbI_3O	monoclinic	70%	-16.9	594
524	NbIO_2	orthorhombic	70%	-12.4	674
525	$\text{NbNi}_5(\text{PO}_4)_6$	trigonal	70%	-7.1	629
526	NbP_2O_7	cubic	100%	-10.6	673
527	$\text{NbP}_6(\text{WO}_8)_3$	trigonal	100%	-7.4	582
528	NbPCl_8O	orthorhombic	70%	-16.8	592
529	NbPO_5	orthorhombic	100%	-11.5	618
530	NbS_2NO_9	orthorhombic	80%	-7.7	679

531	NbV ₂ Fe ₃ (PO ₄) ₆	trigonal	60%	-3.3	629
532	NbV ₂ O ₇	cubic	90%	-8.4	746
533	NbV ₃ (PO ₄) ₆	trigonal	90%	-8.1	714
534	NbV ₃ Cr ₂ (PO ₄) ₆	trigonal	90%	-0.7	693
535	NbV ₃ Cu ₂ (PO ₄) ₆	trigonal	90%	-3.0	700
536	NbV ₃ Fe ₂ (PO ₄) ₆	trigonal	60%	-6.0	623
537	NbV ₅ (PO ₄) ₆	trigonal	70%	-5.0	645
538	NCIO ₄	orthorhombic	60%	-6.6	491
539	Nd(CIO) ₃	orthorhombic	60%	-15.3	1192
540	Nd ₂ Zr ₃ (MoO ₄) ₉	trigonal	80%	-3.9	1113
541	NdGaO ₃	cubic	60%	-12.0	1009
542	NdSeClO ₃	orthorhombic	60%	-9.2	1044
543	Ni(CO) ₄	cubic	80%	-18.6	640
544	Ni(PO ₃) ₄	orthorhombic	80%	-1.2	602
545	Ni ₂ P ₂ O ₉	orthorhombic	70%	-9.4	475
546	Ni ₃ (P ₂ O ₇) ₂	orthorhombic	80%	-9.2	520
547	Ni ₃ (PO ₄) ₄	monoclinic	100%	-9.0	529
548	Ni ₃ P ₄ O ₁₅	orthorhombic	90%	-9.9	552
549	NiAs ₃ H ₃ OF ₁₈	orthorhombic	70%	-13.3	636
550	NiGeH ₁₂ (OF) ₆	trigonal	80%	-22.3	652
551	NiH ₁₂ S ₂ O ₉	orthorhombic	60%	-29.8	569
552	NiMoP ₂ O ₉	orthorhombic	90%	-10.1	660
553	NiP ₂ O ₇	monoclinic	90%	-7.8	429
554	NiP ₂ WO ₉	orthorhombic	70%	-9.7	581
555	NiP ₆ (WO ₈) ₃	trigonal	90%	-7.0	607
556	NiPNO ₁₀	orthorhombic	80%	-6.8	515
557	NiPNO ₅	orthorhombic	90%	-8.5	348
558	NiPO ₄	orthorhombic	100%	-8.9	405
559	NiS ₂ O ₉	orthorhombic	80%	-9.1	540
560	NiSnP ₂ O ₉	orthorhombic	80%	-8.7	545
561	NpNi(OF ₂) ₃	monoclinic	70%	-5.3	1076
562	NpNO ₅	monoclinic	90%	-8.0	987
563	NpPO ₄ F	orthorhombic	70%	-5.2	967
564	Os ₃ O	cubic	70%	-2.3	296
565	Os ₅ Pd(CO) ₁₆	orthorhombic	70%	-17.0	630
566	Os ₆ C ₁₇ SO ₁₇	orthorhombic	70%	-18.0	579
567	Os ₆ C ₁₉ O ₂₀	orthorhombic	70%	-18.4	598

568	Os ₇ C ₁₉ SO ₁₉	monoclinic	60%	-17.4	611
569	OsBr ₂ N ₄ ClO ₂	orthorhombic	60%	-9.1	432
570	OsOF ₅ (Pnma)	orthorhombic	60%	-9.4	460
571	OsOF ₅ (Pna2_1)	orthorhombic	60%	-9.4	457
572	P(W ₃ O ₁₀) ₄	cubic	100%	-13.5	801
573	P ₂ W ₂ O ₁₁	orthorhombic	70%	-10.5	639
574	P ₂ W ₂ O ₉	orthorhombic	90%	-10.5	546
575	P ₂ W ₃ O ₁₃	orthorhombic	70%	-11.0	536
576	P ₂ W ₅ O ₁₉	monoclinic	70%	-4.5	582
577	P ₂ WO ₇	cubic	100%	-11.5	543
578	P ₂ WO ₈	orthorhombic	70%	-7.3	681
579	P ₃ (WO ₆) ₂	trigonal	100%	-6.5	625
580	P ₃ N ₆ O ₇	monoclinic	70%	-15.4	484
581	P ₃ SN ₄ Cl ₅ O	orthorhombic	70%	-17.1	489
582	P ₄ WO ₁₂	orthorhombic	90%	-9.4	676
583	PBr ₃ O	orthorhombic	70%	-12.0	485
584	PCl ₃ O	orthorhombic	80%	-13.7	518
585	PClOF ₂	orthorhombic	80%	-15.6	534
586	Pd ₂ O	cubic	70%	-16.8	224
587	PNO ₃	orthorhombic	80%	-13.3	460
588	PO ₃	orthorhombic	90%	-13.0	552
589	Pr ₂ (MoO ₄) ₃	orthorhombic	80%	-14.6	1171
590	Pr ₂ Hf ₃ (MoO ₄) ₉	trigonal	100%	-13.5	1115
591	PrC ₁₉ S ₆ N ₉ O ₂	monoclinic	60%	-18.3	1180
592	PS ₂ N(Cl ₃ O ₂) ₂	orthorhombic	70%	-14.7	649
593	Pt ₂ O	cubic	60%	-15.7	218
594	PW ₁₂ O ₄₃	cubic	80%	-9.7	820
595	PW ₅ O ₁₇	monoclinic	60%	-9.5	572
596	PWO ₄	orthorhombic	70%	-9.1	572
597	PWO ₅	orthorhombic	90%	-12.0	633
598	Rb ₂ Cd ₂ (MoO ₄) ₃	cubic	60%	-8.2	1210
599	Rb ₂ UH ₂ (SeO ₅) ₂	orthorhombic	60%	-1.3	1050
600	Rb ₃ GaP ₆ (HO ₃) ₆	trigonal	60%	-8.2	1091
601	Rb ₃ P(W ₃ O ₁₀) ₄	cubic	80%	-5.4	1112
602	Rb ₄ Te ₂ S ₈ O ₁₅	orthorhombic	60%	-2.6	1255
603	RbAsOF ₅	orthorhombic	70%	-19.8	1133
604	RbMo ₂ P ₃ O ₁₃	monoclinic	80%	-4.6	1119

605	RbP(OF) ₂	orthorhombic	70%	-0.3	1088
606	Re(Cl ₂ O) ₂	orthorhombic	70%	-13.2	427
607	Re ₂ C ₃ (ClO ₂) ₃	orthorhombic	60%	-16.2	398
608	Re ₃ S ₄ O ₉	trigonal	80%	-16.6	631
609	Re ₃ Se ₄ O ₃	cubic	80%	-16.0	648
610	Re ₃ Se ₄ O ₈ F	monoclinic	70%	-10.0	668
611	ReBi ₃ O ₈	cubic	70%	-16.6	683
612	ReH ₂₂ C ₄ S ₄ N ₈ Cl ₈ O ₃	orthorhombic	60%	-9.9	853
613	ReN ₂ (OF ₄) ₂	orthorhombic	70%	-9.3	423
614	RePCl ₈ O	orthorhombic	80%	-12.1	440
615	ReWO ₆	cubic	90%	-1.0	598
616	RhN ₃ Cl ₆ O	orthorhombic	60%	-18.1	443
617	RhWN ₅ ClO ₄	orthorhombic	70%	-15.2	552
618	Ru(NO ₂) ₆	monoclinic	60%	-6.6	500
619	Ru ₃ C ₁₀ I ₂ O ₉	orthorhombic	70%	-13.7	471
620	RuN ₃ Cl ₃ O	orthorhombic	60%	-17.2	457
621	RuN ₃ Cl ₅ O	orthorhombic	60%	-19.2	449
622	RuN ₄ Cl ₃ O ₂	orthorhombic	60%	-16.1	448
623	RuN ₆ Cl ₃ O ₂	orthorhombic	60%	-20.6	453
624	RuSN ₄ (ClO) ₂	orthorhombic	60%	-20.8	449
625	S(NO ₂) ₂	orthorhombic	70%	-13.4	464
626	S ₂ N(O ₂ F) ₂	monoclinic	60%	-12.3	411
627	Sb(PO ₃) ₄	orthorhombic	90%	-7.3	582
628	Sb ₂ P ₂ O ₉	orthorhombic	90%	-3.8	490
629	Sb ₂ Te ₃ MoC ₄ (OF ₃) ₄	orthorhombic	60%	-10.2	736
630	Sb ₂ Te ₃ WC ₄ (OF ₃) ₄ (Ferromagnetic)	orthorhombic	70%	-9.2	945
631	Sb ₂ Te ₃ WC ₄ (OF ₃) ₄ (Non-magnetic)	orthorhombic	60%	-9.0	726
632	Sb ₃ IO ₄	orthorhombic	60%	-14.2	406
633	Sb ₃ P ₆ WO ₂₄	trigonal	90%	-4.4	668
634	Sb ₄ O ₅ F ₂	orthorhombic	60%	-7.2	395
635	Sb ₈ Cl ₂ O ₁₅	monoclinic	70%	-9.8	287
636	SbH ₈ C ₂ S ₂ Br ₃ N ₄ O	orthorhombic	60%	-20.7	585
637	SbO ₂	hexagonal	60%	-11.4	413
638	SbOF	orthorhombic	60%	-8.7	246
639	SbP ₆ (WO ₈) ₃	trigonal	90%	-3.8	636
640	SbPC ₃ Cl ₅ O	orthorhombic	60%	-15.8	456
641	SbPCl ₈ O	orthorhombic	80%	-12.4	464

642	SbS ₈ Cl ₅ O	orthorhombic	60%	-17.1	646
643	SbTeClO ₃	orthorhombic	60%	-11.6	402
644	Se ₂ S ₈ N ₄ O ₁₅	orthorhombic	90%	-12.9	624
645	Si(Sn ₃ O ₄) ₂	hexagonal	70%	-14.4	592
646	Si ₁₆ O ₃₂ F	monoclinic	70%	-17.7	551
647	Si ₃ (Cl ₄ O) ₂	orthorhombic	70%	-16.3	576
648	Si ₉ C ₄ NO ₁₈	monoclinic	80%	-18.3	786
649	SiMoP ₃ O ₁₁	trigonal	100%	-4.3	736
650	SiN ₄ (OF ₂) ₃	hexagonal	60%	-12.4	580
651	SiP ₃ RuO ₁₁	trigonal	80%	-3.1	751
652	Sm(ReO ₅) ₃	orthorhombic	100%	-13.6	1085
653	SmAgO ₂	hexagonal	60%	-13.2	981
654	SmRe ₃ O ₁₆	orthorhombic	100%	-13.9	1083
655	SmSeClO ₃	orthorhombic	90%	-9.8	1002
656	Sn(PO ₃) ₄	orthorhombic	80%	-6.6	589
657	Sn ₂ C ₆ N ₂ O ₁₇	orthorhombic	90%	-17.7	600
658	Sn ₃ (OF) ₂	orthorhombic	80%	-17.3	415
659	SN ₄ O ₅	orthorhombic	70%	-13.1	475
660	Sn ₄ P ₂ O ₉	orthorhombic	70%	-6.9	405
661	Sn ₅ P ₆ O ₂₅	trigonal	70%	-2.8	536
662	Sn ₆ P ₃ NO ₁₄	orthorhombic	80%	-15.3	415
663	SnH ₄ (Cl ₂ O) ₂	orthorhombic	60%	-20.5	550
664	SnN ₂ Cl ₄ O	orthorhombic	70%	-11.1	417
665	SnO ₂	hexagonal	60%	-14.3	398
666	SNO ₃ F	orthorhombic	60%	-13.0	467
667	SnP ₆ (WO ₈) ₃	trigonal	90%	-3.4	601
668	SnPClO ₂	orthorhombic	70%	-10.9	438
669	SnPO ₄	orthorhombic	90%	-3.8	473
670	SnWO ₄	cubic	90%	-19.8	489
671	Sr ₂ V ₂ OF ₁₀	orthorhombic	60%	-16.7	1173
672	SrBr ₂ O	orthorhombic	70%	-26.8	1158
673	SrCd(IO ₂) ₄	orthorhombic	70%	-23.5	1197
674	SrI ₂ O	orthorhombic	60%	-25.9	1135
675	SrIO	orthorhombic	60%	-25.2	1139
676	SrMn ₂ O ₁₁	cubic	70%	-1.9	1133
677	SrP ₃ NO ₁₂	orthorhombic	60%	-7.0	1127
678	Ta(PO ₄) ₂	orthorhombic	90%	-10.4	643

679	Ta ₁₂ MoO ₃₃	monoclinic	60%	-4.1	709
680	Ta ₂ Cd(P ₂ O ₇) ₃	orthorhombic	80%	-10.9	636
681	Ta ₂ W ₂ O ₁₁	monoclinic	90%	-14.9	484
682	Ta ₃ Sb(PO ₄) ₆	trigonal	90%	-7.6	621
683	Ta ₇ (P ₂ O ₇) ₈	trigonal	90%	-1.3	710
684	TaAsO ₅	orthorhombic	60%	-9.9	607
685	TaNbO ₅	orthorhombic	90%	-12.6	688
686	TaNiP ₂ O ₉	orthorhombic	70%	-9.9	562
687	TaO ₃	cubic	90%	-4.5	522
688	TaP ₂ O ₇	cubic	100%	-10.7	544
689	TaSCl ₇ O	orthorhombic	80%	-13.6	547
690	Tb ₂ (MoO ₄) ₃	orthorhombic	90%	-18.8	1181
691	Tb ₂ (SO ₄) ₃	orthorhombic	80%	-8.8	1089
692	Tb ₂ (WO ₄) ₃	orthorhombic	100%	-19.9	1129
693	TbSeClO ₃	orthorhombic	90%	-9.7	996
694	TcBi ₃ O ₈	cubic	70%	-17.0	683
695	Te ₂ W(NO ₄) ₂	monoclinic	70%	-5.6	634
696	Te ₃ C ₂ S ₂ (OF) ₆	monoclinic	60%	-4.9	464
697	Te ₃ H ₄ (NO ₆) ₂	orthorhombic	70%	-1.4	581
698	Te ₃ Mo ₅ O ₁₈	monoclinic	80%	-0.4	723
699	Te ₃ W ₅ O ₁₈	monoclinic	70%	-4.4	680
700	Te ₄ As ₂ S(OF ₆) ₂	orthorhombic	80%	-9.1	494
701	Th ₂ N ₇ OF ₁₅	cubic	60%	-17.0	1307
702	Th ₂ P ₃ O ₁₃	monoclinic	60%	-6.9	1095
703	Ti(PO ₃) ₄	orthorhombic	60%	-0.5	667
704	Ti(PO ₄) ₂	monoclinic	80%	-16.9	608
705	Ti ₂ C ₂ O ₉	orthorhombic	60%	-10.2	596
706	Ti ₂ Cu(PO ₄) ₃	trigonal	60%	-0.7	554
707	Ti ₂ Sb(PO ₄) ₃	trigonal	60%	-5.2	601
708	Ti ₂ Sn(PO ₄) ₃	trigonal	70%	-3.9	657
709	Ti ₃ Co ₂ P ₆ WO ₂₄	trigonal	60%	-5.1	636
710	Ti ₃ Co ₂ Te(PO ₄) ₆	trigonal	60%	-5.4	602
711	Ti ₃ CoSn ₂ (PO ₄) ₆	trigonal	70%	-4.5	657
712	Ti ₃ Cr(PO ₄) ₆	trigonal	80%	-7.9	676
713	Ti ₃ Cr ₂ Fe(PO ₄) ₆	trigonal	70%	-0.2	695
714	Ti ₃ Cr ₂ Sb(PO ₄) ₆	trigonal	80%	-0.7	723
715	Ti ₃ Cr ₂ Sn(PO ₄) ₆	trigonal	80%	-0.3	728

716	Ti ₃ CrSb ₂ (PO ₄) ₆	trigonal	70%	-5.9	645
717	Ti ₃ CrSn ₂ (PO ₄) ₆	trigonal	60%	-5.0	697
718	Ti ₃ Cu ₂ P ₆ WO ₂₄	trigonal	90%	-2.8	661
719	Ti ₃ Cu ₂ Sb(PO ₄) ₆	trigonal	80%	-2.9	557
720	Ti ₃ Cu ₂ Sn(PO ₄) ₆	trigonal	80%	-2.9	582
721	Ti ₃ Cu ₂ Te(PO ₄) ₆	trigonal	80%	-3.0	560
722	Ti ₃ CuSn ₂ (PO ₄) ₆	trigonal	60%	-5.5	596
723	Ti ₃ Fe ₂ P ₆ WO ₂₄	trigonal	60%	-6.1	581
724	Ti ₃ Fe ₂ Sb(PO ₄) ₆	trigonal	60%	-6.1	689
725	Ti ₃ Fe ₂ Sn(PO ₄) ₆	trigonal	60%	-6.2	683
726	Ti ₃ Fe ₂ Te(PO ₄) ₆	trigonal	70%	-6.4	686
727	Ti ₃ FeCu ₂ (PO ₄) ₆	trigonal	80%	-0.8	712
728	Ti ₃ FeSb ₂ (PO ₄) ₆	trigonal	60%	-5.0	694
729	Ti ₃ FeSn ₂ (PO ₄) ₆	trigonal	60%	-5.6	746
730	Ti ₃ Mn ₂ Nb(PO ₄) ₆	trigonal	70%	-0.7	718
731	Ti ₃ Mn ₂ P ₆ WO ₂₄	trigonal	70%	-1.9	666
732	Ti ₃ MnCr(PO ₄) ₆	trigonal	70%	-3.1	728
733	Ti ₃ MnSb ₂ (PO ₄) ₆	trigonal	60%	-3.8	608
734	Ti ₃ MnSn ₂ (PO ₄) ₆	trigonal	60%	-3.6	654
735	Ti ₃ Nb ₂ Cr(PO ₄) ₆	trigonal	80%	-1.9	684
736	Ti ₃ NbCo ₂ (PO ₄) ₆	trigonal	60%	-3.9	690
737	Ti ₃ NbCu ₂ (PO ₄) ₆	trigonal	80%	-1.4	710
738	Ti ₃ NbFe ₂ (PO ₄) ₆	trigonal	60%	-3.2	696
739	Ti ₃ NbNi ₂ (PO ₄) ₆	trigonal	60%	-4.4	644
740	Ti ₃ NbV ₂ (PO ₄) ₆	trigonal	70%	-1.6	685
741	Ti ₃ P ₄ (NO ₈) ₂	monoclinic	70%	-8.8	549
742	Ti ₃ P ₄ (NO ₉) ₂	monoclinic	60%	-8.4	570
743	Ti ₃ P ₆ WO ₂₄	trigonal	100%	-8.3	662
744	Ti ₃ Sb ₂ (PO ₄) ₆	trigonal	70%	-0.4	608
745	Ti ₃ V ₂ P ₆ WO ₂₄	trigonal	70%	-6.2	577
746	Ti ₃ VSb ₂ (PO ₄) ₆	trigonal	60%	-6.0	694
747	Ti ₃ VSn ₂ (PO ₄) ₆	trigonal	60%	-5.1	732
748	Ti ₄ P ₆ PbO ₂₄	trigonal	80%	-6.2	619
749	Ti ₆ In ₂ Si ₂ P ₁₂ O ₄₉	trigonal	70%	-8.4	728
750	TiC ₇ (NO) ₁₂	monoclinic	70%	-18.9	631
751	TiCr ₃ (PO ₄) ₆	trigonal	90%	-7.8	682
752	TiFe ₃ Sb ₂ (PO ₄) ₆	trigonal	60%	-6.3	699

753	TiMn ₂ Fe ₃ (PO ₄) ₆	trigonal	60%	-0.3	677
754	TiMn ₃ Cu ₂ (PO ₄) ₆	trigonal	70%	-0.8	533
755	TiNb ₃ (PO ₄) ₆	trigonal	90%	-7.8	690
756	TiNiP ₂ O ₉	orthorhombic	70%	-9.6	581
757	TiOF ₂	monoclinic	60%	-15.4	466
758	TiP ₂ H ₂ O ₉	monoclinic	60%	-3.5	872
759	TiP ₂ O ₇	cubic	80%	-8.5	550
760	TiP ₆ (WO ₈) ₃	trigonal	100%	-7.3	582
761	TiV ₂ O ₇	cubic	80%	-9.9	763
762	TiV ₃ Cu ₂ (PO ₄) ₆	trigonal	80%	-1.2	688
763	TiV ₃ Sn ₂ (PO ₄) ₆	trigonal	60%	-5.5	694
764	Tl ₂ Ni ₂ (MoO ₄) ₃	cubic	60%	-9.0	932
765	Tl ₃ (MoO ₄) ₂	hexagonal	60%	-16.4	610
766	Tl ₃ Hg ₂ S ₃ ClO ₁₂	monoclinic	60%	-15.4	392
767	TlFeC ₃ NO ₄	cubic	60%	-11.5	655
768	TlMo ₂ P ₃ O ₁₃	monoclinic	80%	-8.6	652
769	TlPO ₃	orthorhombic	60%	-0.2	615
770	TmSeClO ₃	orthorhombic	80%	-10.1	993
771	TmTl(MoO ₄) ₂	orthorhombic	60%	-15.1	1028
772	U(ClO) ₂	orthorhombic	60%	-15.2	1116
773	U(MoO ₅) ₁₂	trigonal	80%	-7.3	1192
774	U ₂ O ₅ F ₈	orthorhombic	80%	-16.0	1182
775	U ₂ PCl ₁₁ O	orthorhombic	70%	-16.2	1200
776	U ₂ S(NO ₅) ₂	orthorhombic	90%	-8.6	1068
777	U ₂ Tl ₂ Mo ₃ O ₁₆	orthorhombic	80%	-17.2	982
778	U ₂ V ₂ NiO ₁₆	orthorhombic	80%	-3.9	1082
779	U ₃ (PO ₉) ₂	orthorhombic	100%	-8.5	1080
780	U ₃ O ₁₁	orthorhombic	90%	-13.4	974
781	UBCO ₅	orthorhombic	60%	-31.1	1079
782	UC ₂ O ₇	orthorhombic	70%	-15.2	1089
783	UC ₂ Se ₂ (NO ₆) ₂	orthorhombic	80%	-11.5	1150
784	UC ₄ O ₇	orthorhombic	60%	-9.4	1072
785	UCrO ₉	monoclinic	100%	-8.1	1039
786	UCu(Mo ₂ O ₉) ₆	trigonal	70%	-6.6	1192
787	UN ₂ O ₇	orthorhombic	70%	-19.1	1074
788	UO ₃	cubic	80%	-17.0	945
789	UPO ₅	orthorhombic	70%	-1.2	950

790	UV ₂ O ₈	orthorhombic	90%	-9.3	1055
791	V(Bi ₅ O ₈) ₅	monoclinic	60%	-8.3	658
792	V(PO ₃) ₄	orthorhombic	80%	-2.6	758
793	V ₂ (PO ₄) ₃	trigonal	60%	-8.4	660
794	V ₂ AgP ₃ O ₁₁	monoclinic	80%	-4.7	522
795	V ₂ CoO ₈	orthorhombic	60%	-9.3	599
796	V ₂ CrO ₇	cubic	70%	-2.7	699
797	V ₂ Cu(PO ₄) ₃	trigonal	90%	-2.1	644
798	V ₂ Fe ₃ P ₆ WO ₂₄	trigonal	70%	-2.9	642
799	V ₂ Fe ₃ Sb(PO ₄) ₆	trigonal	60%	-3.1	638
800	V ₂ Fe ₃ Sn(PO ₄) ₆	trigonal	60%	-6.5	583
801	V ₂ Hg ₂ O ₇	orthorhombic	80%	-12.3	618
802	V ₂ NiO ₈	orthorhombic	60%	-8.8	628
803	V ₂ O ₅	orthorhombic	70%	-8.9	784
804	V ₂ P ₂ O ₉	orthorhombic	80%	-10.3	623
805	V ₂ SnO ₇	cubic	100%	-7.6	560
806	V ₂ SO ₈	orthorhombic	70%	-9.3	597
807	V ₃ (PO ₄) ₄	monoclinic	90%	-6.9	716
808	V ₃ Bi ₂ (PO ₄) ₆	trigonal	80%	-1.2	612
809	V ₃ Co ₂ P ₆ WO ₂₄	trigonal	60%	-4.4	580
810	V ₃ CoSb ₂ (PO ₄) ₆	trigonal	60%	-7.4	612
811	V ₃ CoSn ₂ (PO ₄) ₆	trigonal	60%	-7.4	612
812	V ₃ Cr(PO ₄) ₆	trigonal	80%	-7.7	656
813	V ₃ Cr ₂ Sn(PO ₄) ₆	trigonal	90%	-2.2	659
814	V ₃ CrSb ₂ (PO ₄) ₆	trigonal	60%	-7.3	662
815	V ₃ CrSn ₂ (PO ₄) ₆	trigonal	60%	-7.0	661
816	V ₃ Cu(PO ₄) ₆	trigonal	80%	-7.6	636
817	V ₃ Cu ₂ Ni(PO ₄) ₆	trigonal	90%	-3.3	591
818	V ₃ Cu ₂ P ₆ WO ₂₄	trigonal	90%	-4.4	589
819	V ₃ Cu ₂ Sb(PO ₄) ₆	trigonal	90%	-3.3	601
820	V ₃ Cu ₂ Sn(PO ₄) ₆	trigonal	90%	-3.3	610
821	V ₃ Cu ₂ Te(PO ₄) ₆	trigonal	90%	-4.2	603
822	V ₃ Fe ₂ Sb(PO ₄) ₆	trigonal	60%	-7.3	595
823	V ₃ Fe ₂ Te(PO ₄) ₆	trigonal	60%	-7.5	595
824	V ₃ Ni(PO ₄) ₆	trigonal	60%	-7.6	638
825	V ₃ Ni ₂ P ₆ WO ₂₄	trigonal	70%	-6.4	586
826	V ₃ P ₄ O ₁₅	orthorhombic	90%	-10.5	714

827	$V_3P_4WO_{20}$	monoclinic	70%	-11.1	690
828	$V_3P_6WO_{24}$	trigonal	100%	-8.4	661
829	$V_3S_2NO_{12}$	monoclinic	70%	-7.3	609
830	$V_3Sb(PO_4)_6$	trigonal	70%	-4.7	656
831	$V_3Sb_2(PO_4)_6$	trigonal	70%	-2.9	689
832	$V_4(P_2O_7)_3$	orthorhombic	90%	-10.7	698
833	V_4CuNiO_{12}	monoclinic	80%	-0.3	550
834	$V_5P_6WO_{24}$	trigonal	70%	-4.3	578
835	$V_5Sb(PO_4)_6$	trigonal	60%	-5.4	592
836	$VAsO_5$	orthorhombic	70%	-5.5	491
837	$VCdClO_3$	orthorhombic	80%	-12.8	596
838	$VCdPO_7$	monoclinic	80%	-7.7	497
839	$VCo(PO_4)_2$	trigonal	60%	-5.6	596
840	$VCr_3(PO_4)_6$	trigonal	90%	-7.8	669
841	$VFe_3Sb_2(PO_4)_6$	trigonal	60%	-7.4	622
842	$VHg_4P_2O_9$	orthorhombic	60%	-16.8	561
843	$VNi_3Sb_2(PO_4)_6$	trigonal	60%	-7.4	611
844	$VNiP_2O_9$	orthorhombic	80%	-10.2	616
845	VP_2O_7	monoclinic	80%	-10.5	617
846	$VP_6(WO_8)_3$	trigonal	100%	-7.2	579
847	VPN_2O_5	monoclinic	80%	-16.6	558
848	$VPNO_6$	monoclinic	90%	-9.3	545
849	VPO_5	orthorhombic	90%	-10.5	708
850	VSO_4F_3	orthorhombic	70%	-6.6	637
851	$VZnPbO_5$	orthorhombic	60%	-11.6	658
852	$W(CO)_6$	orthorhombic	70%	-18.5	565
853	$W_3C_7NCl_6O_7$	orthorhombic	70%	-17.9	786
854	W_3O_8	hexagonal	70%	-8.5	607
855	$W_7(OF_5)_6$	trigonal	80%	-6.8	584
856	$WN_2(OF_2)_2$	monoclinic	60%	-10.0	520
857	$WN_2(OF_4)_2$	orthorhombic	70%	-9.9	578
858	WO_2	hexagonal	70%	-8.1	748
859	WO_3	cubic	90%	-10.5	491
860	$Y(PO_3)_3$	trigonal	70%	-6.7	1216
861	$Y_2(SeO_4)_3$	orthorhombic	100%	-2.7	1139
862	$Y_2(SO_4)_3$	orthorhombic	60%	-4.5	1162
863	$YAgO_2$	hexagonal	70%	-11.0	1032

864	Yb(PO ₃) ₃	trigonal	90%	-8.0	1132
865	Yb ₄ Br ₆ O	hexagonal	70%	-16.3	1095
866	YbI ₂ O	orthorhombic	60%	-18.8	1087
867	YbP ₃ O ₁₀	monoclinic	90%	-6.4	1038
868	YbSeClO ₃	orthorhombic	90%	-9.1	973
869	YbTl(MoO ₄) ₂	orthorhombic	60%	-16.2	1008
870	YSeClO ₃	orthorhombic	70%	-26.9	1084
871	Zn ₂ MoSeO ₇	monoclinic	60%	-5.6	510
872	Zn ₂ P ₃ C(NO ₄) ₃	monoclinic	70%	-15.1	458
873	Zn ₂ SiO ₄	trigonal	80%	-1.9	381
874	Zn ₂ TeMoO ₇	monoclinic	60%	-2.4	565
875	Zn ₃ (PO ₆) ₂	orthorhombic	90%	-7.2	435
876	Zn ₄ As ₃ C ₃ N ₃ O ₁₃	monoclinic	70%	-13.2	420
877	Zn ₄ P ₃ C ₃ N ₃ O ₁₃	monoclinic	70%	-13.8	461
878	ZnAsNO ₄	monoclinic	70%	-10.6	390
879	ZnAsWO ₅	monoclinic	70%	-12.2	510
880	ZnBi ₂ P ₂ O ₉	orthorhombic	60%	-1.8	477
881	ZnC ₂ S ₂ (OF) ₆	trigonal	60%	-6.0	507
882	ZnCr ₂ O ₇	monoclinic	70%	-0.1	580
883	ZnCuP ₂ O ₇	monoclinic	100%	-4.3	175
884	ZnFe ₂ (P ₂ O ₇) ₂	orthorhombic	80%	-9.8	707
885	ZnFe ₂ (PO ₄) ₂	monoclinic	80%	-3.3	534
886	ZnMo ₂ O ₇	monoclinic	90%	-10.0	589
887	ZnMo ₂ P ₂ O ₉	orthorhombic	80%	-9.0	602
888	ZnMo ₃ O ₇	orthorhombic	70%	-8.6	696
889	ZnMoAsO ₅	monoclinic	60%	-4.4	511
890	ZnMoO ₆	monoclinic	90%	-9.0	688
891	ZnNiMoP ₂ O ₉	orthorhombic	90%	-7.0	576
892	ZnNiSnP ₂ O ₉	orthorhombic	60%	-4.7	293
893	ZnP ₂ (WO ₅) ₂	orthorhombic	60%	-6.0	515
894	ZnP ₂ W ₂ O ₉	orthorhombic	60%	-8.3	570
895	ZnPNO ₄	monoclinic	80%	-6.7	425
896	ZnSn ₂ P ₂ O ₉	orthorhombic	70%	-5.8	437
897	ZnSnAsO ₅	monoclinic	70%	-4.8	241
898	ZnW ₂ O ₇	monoclinic	90%	-16.4	503
899	Zr(AsO ₅) ₂	monoclinic	70%	-2.4	557
900	Zr(PO ₅) ₂	monoclinic	70%	-3.8	681

901	Zr ₂ (PO ₄) ₃	trigonal	80%	-3.7	740
902	Zr ₂ Ga(PO ₄) ₃	trigonal	70%	-3.0	760
903	Zr ₄ Cd(PO ₄) ₆	trigonal	80%	-0.6	759
904	ZrFe(PO ₄) ₃	orthorhombic	70%	-10.9	729
905	ZrO ₃ F ₅	orthorhombic	60%	-0.5	969
906	ZrP ₂ CO ₆	monoclinic	60%	-8.1	493
907	ZrP ₂ N ₃ O ₈ F	monoclinic	60%	-12.3	889
908	ZrP ₂ O ₇	cubic	100%	-9.6	619

Table S2 NTE prediction set (Cyanides). T2 is the upper temperature limit, and the lower temperature limit is uniformly set as 0K. NTE is set to one decimal place, T2 to an integer.

No.	Formula	Crystal System	Probability (%)	NTE (ppm/K)	T2(K)
1	((C H ₃) C Cl ₃) Cd (C N) ₂	cubic	60%	-27.5	773
2	((C H ₃) ₄ N) (Cu Zn (C N) ₄)	cubic	60%	-6.2	840
3	((C H ₃) ₄ N) ₂ Mn (Cl ₁₂ (Nb (C N)) ₆)	cubic	60%	-6.2	683
4	((Co (H ₂ O) ₂) ₂ Mo (C N) ₈) (H ₂ O) ₄	tetragonal	60%	-8.8	521
5	((N (C H ₃) ₄) (Cu Zn (C N) ₄)) (C Cl ₄) _{0.9}	cubic	80%	-3.8	835
6	(Cd (C N) ₂) (C (C H ₃) ₂ Cl ₂)	cubic	60%	-9.6	813
7	(Cd (C N) ₂) (C Cl ₄)	cubic	60%	-26.9	817
8	(Cd Hg (C N) ₄) (C Cl ₄) ₂	cubic	70%	-15.4	811
9	(Cd Zn (C N) ₄) (C Cl ₄) ₂	cubic	60%	-28.6	812
10	(Cd ₃ (Co _{0.5} Cr _{0.5} (C N) ₆) ₂ (H ₂ O) ₁₅) _{1.3333}	cubic	60%	-28.0	320
11	(Co ₃ Fe ₂ (C N) ₁₂ (H ₂ O) ₁₄) _{1.33}	cubic	60%	-26.1	319
12	(Cu (H ₂ O) ₂) ₂ (Mo (C N) ₈) (H ₂ O) ₂	tetragonal	60%	-24.0	446
13	(La _{0.75} Pr _{0.25}) Co (C N) ₆ (H ₂ O) ₅	hexagonal	60%	-11.0	439
14	Al (C N) ₃	cubic	60%	-3.3	504
15	Am (Ag (C N) ₂) ₃ (H ₂ O) ₃	hexagonal	60%	-7.9	301
16	Be (C N) ₂	cubic	90%	-9.4	453
17	C ₈ H ₁₂ Mn ₂ Mo N ₁₂ O ₅	tetragonal	60%	-36.0	538
18	Ca K ₄ (Re ₃ Mo ₃ S ₈ (C N) ₆) (H ₂ O) ₈	cubic	60%	-9.8	725
19	Cd (Cr _{0.333} Ir _{0.333} (C N) ₄) (H ₂ O) _{4.333}	cubic	60%	-11.9	320
20	Cd ₄ ((Fe _{1.333} Co _{1.333}) (C N) ₁₆) (H ₂ O) _{18.667}	cubic	60%	-38.1	319
21	Co (Co _{0.333} Ir _{0.333} (C N) ₄) (H ₂ O) _{4.333}	cubic	60%	-32.3	337
22	Cs _{2.75} K _{1.25} (Re ₆ Se ₈ (C N) ₄ (O H) ₂) (H ₂ O)	tetragonal	60%	-14.4	858
23	Cs ₆ ((Re ₆ (C N) ₃ S ₈) ₂ S C)	hexagonal	60%	-18.2	815
24	Fe (Co _{0.2} Fe _{0.8} (C N) ₆)	cubic	100%	-11.1	443
25	Fe (Fe _{0.97} (C N) ₆) _{0.88} (H ₂ O) _{0.473}	cubic	60%	-8.7	463

26	$\text{Fe}_4 \text{Fe}_{3-00} (\text{C N})_{18-0} (\text{H}_2 \text{O})_{11-0}$	cubic	60%	-41.8	715
27	$\text{Ga} (\text{C N})_3$	cubic	90%	-8.1	387
28	$\text{H}_{0.2} (\text{Ru}_2 (\text{O}_2 \text{C} (\text{C H}_3))_4)_{2-8} (\text{Cr} (\text{C N})_5 \text{N O})$	cubic	60%	-0.6	684
29	$\text{In} (\text{C N})_3$	cubic	80%	-21.9	383
30	$\text{In}_{0-08} \text{Eu}_4 (\text{N C N})_3 \text{I}_3$	hexagonal	60%	-2.3	600
31	$\text{K Cu} ((\text{Co}_{0.7} \text{Fe}_{0.3}) (\text{C N})_6)$	cubic	60%	-7.6	264
32	$\text{K}_{1.9} (\text{Fe}_4 \text{Fe}_{3-00} (\text{C N})_{18-00}) ((\text{O H})_{1.9} (\text{H}_2 \text{O})_{7-0})$	cubic	60%	-4.7	784
33	$\text{K}_6 (\text{Mo}_3 \text{Re}_3 \text{S}_8 (\text{C N})_5)$	tetragonal	60%	-6.6	553
34	$\text{K}_6 (\text{Se}_8 (\text{Mo}_6 (\text{C N})_5))$	tetragonal	60%	-9.7	603
35	$\text{Li Eu}_2 (\text{N C N}) \text{I}_3$	cubic	60%	-28.5	757
36	$\text{Mn} (\text{C N})_2$	cubic	90%	-33.3	442
37	$\text{Na}_{0.5} \text{Fe} (\text{Fe} (\text{C N})_6)$	cubic	90%	-8.5	448
38	$\text{Na}_{0.52} \text{Fe} (\text{Fe} (\text{C N})_6)$	cubic	90%	-7.3	447
39	$\text{Na}_{0.55} \text{Fe} (\text{Fe} (\text{C N})_6)$	cubic	90%	-12.9	446
40	$\text{Nd} (\text{Ag} (\text{C N})_2)_3 (\text{H}_2 \text{O})_3$	hexagonal	60%	-7.7	305
41	$\text{Ni} (\text{C N})_2 (\text{N H}_3)$	tetragonal	60%	-4.4	390
42	$\text{Pd} (\text{C N})_2$	tetragonal	60%	-8.1	317
43	$\text{Pr} (\text{Ag} (\text{C N})_2)_3 (\text{H}_2 \text{O})_3$	hexagonal	60%	-7.7	302
44	$\text{Pr Co} (\text{C N})_6 (\text{H}_2 \text{O})_5$	hexagonal	60%	-11.1	440
45	$\text{Pt} (\text{C N})_2$	tetragonal	60%	-2.2	346
46	Tl C N	cubic	60%	-11.1	283
47	$\text{Zn}[\text{N}(\text{CN})_2]_2$	orthorhombic	80%	-11.8	431

Table S3 NTE prediction set (Fluorides). T2 is the upper temperature limit, and the lower temperature limit is uniformly set as 0K. NTE is set to one decimal place, T2 to an integer.

No.	Formula	Crystal System	Probability (%)	NTE (ppm/K)	T2(K)
1	AcF_3	cubic	90%	-28.2	375
2	$\text{Ba}_{18}\text{In}_8(\text{S}_7\text{F}_6)_3$	tetragonal	60%	-19.1	873
3	$\text{Ba}_3\text{Ti}_2(\text{O}_3\text{F}_5)_2$	tetragonal	60%	-10.5	698
4	BaTaF_7	cubic	70%	-3.0	990
5	BNF_8	tetragonal	60%	-11.4	419
6	CaSnF_4	tetragonal	60%	-21.9	399
7	CaSnF_6	cubic	100%	-6.2	200
8	CaTbF_6	tetragonal	60%	-22.8	650
9	$\text{CrRu}(\text{NF})_6$	cubic	60%	-9.0	973
10	$\text{Cs}_2\text{SCL}_6\text{F}$	cubic	60%	-7.2	576
11	CsCu_2F_6	cubic	60%	-12.5	548

12	Cu ₂ OF ₂	tetragonal	60%	-5.6	518
13	Cu ₄ OF ₆	tetragonal	60%	-10.0	555
14	Fe(NF ₂) ₃	cubic	60%	-10.2	467
15	GdF ₃	cubic	70%	-25.5	544
16	HfFeF ₆	cubic	90%	-11.3	737
17	HfMnF ₆	cubic	90%	-17.9	745
18	HfTiF ₆	cubic	100%	-16.7	500
19	HfVF ₆	cubic	100%	-8.3	738
20	Hg ₃ F	cubic	60%	-24.3	313
21	K ₂ AgAsF ₆	cubic	60%	-3.6	585
22	K ₂ AgSbF ₆	cubic	60%	-3.1	591
23	K ₂ CuSbF ₆	cubic	60%	-3.6	585
24	KHo ₃ F ₁₀	cubic	60%	-13.7	972
25	KTb ₃ F ₁₀	cubic	60%	-15.7	956
26	KY ₃ F ₁₀	cubic	60%	-15.5	959
27	LaF ₃	cubic	70%	-33.0	319
28	LiVF ₆	cubic	80%	-26.1	364
29	LuF ₃	cubic	90%	-24.4	377
30	Mn ₂ Hg ₂ SF ₆	cubic	60%	-9.8	637
31	MoF ₃	cubic	60%	-7.5	442
32	NaSc(NF ₃) ₂	cubic	80%	-23.1	369
33	NaTh ₂ F ₉	tetragonal	60%	-2.3	651
34	NaUF ₆	cubic	60%	-6.3	644
35	NaV(NF ₃) ₂	cubic	70%	-16.0	401
36	NbF ₃	cubic	90%	-7.8	471
37	NpF ₅	tetragonal	60%	-5.8	560
38	PNF ₆	cubic	80%	-21.6	442
39	Pt ₃ F	cubic	70%	-9.9	359
40	Rb ₂ CuAsF ₆	cubic	60%	-3.0	595
41	Rb ₂ SCl ₆ F	cubic	70%	-12.2	534
42	Rb ₅ Nb ₃ OF ₁₈	tetragonal	70%	-8.6	676
43	RbEu ₃ F ₁₀	cubic	60%	-15.8	972
44	RbTb ₃ F ₁₀	cubic	60%	-15.7	957
45	ReC ₃ O ₄ F	tetragonal	80%	-10.0	715
46	Sc(NF ₂) ₃	cubic	60%	-11.7	467
47	ScC ₃ (N ₃ F ₂) ₃	cubic	70%	-39.2	1074
48	Si(NF ₃) ₂	cubic	60%	-8.5	470
49	SiF ₄	cubic	60%	-15.3	501

50	SNF	tetragonal	80%	-31.9	541
51	SrAlF ₅	tetragonal	60%	-15.6	992
52	SrCrF ₅	tetragonal	80%	-9.6	673
53	SrPdF ₄	tetragonal	60%	-10.0	544
54	TaAgF ₆	tetragonal	90%	-0.4	364
55	TaCl ₄ F	tetragonal	90%	-11.3	711
56	TaF ₃	cubic	100%	-13.4	402
57	TbCd ₂ F ₈	tetragonal	60%	-12.9	561
58	TbCdF ₆	tetragonal	60%	-12.8	558
59	Ti(NF ₂) ₃	cubic	60%	-10.8	469
60	TiCuNO ₄ F ₇	tetragonal	70%	-20.3	392
61	TiF ₂	cubic	80%	-13.6	573
62	TiF ₃	cubic	60%	-8.8	625
63	TiZnF ₄	tetragonal	80%	-12.9	329
64	Tl ₂ VF ₆	cubic	60%	-1.7	699
65	TmF ₃	cubic	80%	-24.1	383
66	UF ₃	cubic	60%	-26.5	521
67	UF ₅	tetragonal	60%	-6.3	559
68	UOF ₄	tetragonal	70%	-3.7	654
69	V(NF ₂) ₃	cubic	70%	-0.6	488
70	V(NF ₃) ₂	cubic	70%	-8.7	479
71	VF ₅	tetragonal	70%	-23.6	559
72	VRu(NF) ₆	cubic	60%	-8.0	966
73	WO ₂ F	tetragonal	100%	-14.8	472
74	WOF ₄	tetragonal	90%	-1.0	482
75	Y ₃ NF ₁₀	cubic	90%	-14.0	1001
76	YbF ₃	cubic	80%	-19.4	415
77	YF ₃	cubic	60%	-26.3	516
78	Zn(NF ₂) ₂	tetragonal	60%	-3.9	473
79	Zr ₃ Pb(O ₂ F ₃) ₂	cubic	60%	-3.1	635
80	ZrCrF ₆	cubic	80%	-5.0	647
81	ZrTiF ₆	cubic	100%	-23.0	586
82	ZrVF ₆	cubic	100%	-4.1	647