

Supporting Materials

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

Yu Cai^{a,b}, Chunyan Wang^{a,b,c}, Huanli Yuan^c, Yuan Guo^{a,e}, Jun-Hyung Cho^d, Xianran Xing^{e,*},
Yu Jia^{*,a,b,f}

^a Key Laboratory for Special Functional Materials of Ministry of Education, and School of Materials and Engineering, Henan University, Kaifeng 475001, China

^b Institute of Quantum Materials and Physics, Henan Academy of Sciences, Zhengzhou 450046, China

^c School of Physics and Telecommunication Engineering, Zhoukou Normal University, Zhoukou 466001, China

^dDepartment of Physics and Research Institute for Natural Science, Hanyang University, 222 Wangsimni-ro, Seongdong-Ku, Seoul 04763, Republic of Korea

^e Institute of Solid States Chemistry, University of Science and Technology Beijing, Beijing 100083, China

^f Joint center for Theoretical Physics, and School of Physics and Electronics, Henan University, Kaifeng 475001, China

Table S1 Thermal expansion training sets. T2 is the upper temperature limit, and the lower temperature limit is uniformly set as 0K. Coefficient of thermal expansion (CTE) is set to one decimal place, T2 to an integer.

No.	Formula	Crystal System	CTE (ppm/K)	T2(K)	Reference
1	Sc ₂ Mo ₃ O ₁₂	orthorhombic	-6.3	300	1
2	In _{0.5} Sc _{1.5} (MoO ₄) ₃	orthorhombic	-3.8	973	2
3	Sc _{1.5} Zr _{0.5} Mo _{2.5} V _{0.5} O ₁₂	orthorhombic	-2.4	673	3
4	Cr _{0.5} ScZr _{0.5} Mo _{2.5} V _{0.5} O ₁₂	orthorhombic	-1.2	673	3
5	Cr _{0.8} Sc _{0.7} Zr _{0.5} Mo _{2.5} V _{0.5} O ₁₂	orthorhombic	-0.2	673	3
6	La ₂ Mo ₃ O ₁₂	monoclinic	19.1	1073	4
7	Er ₂ Mo ₃ O ₁₂	orthorhombic	-22.7	1073	4
8	Yb ₂ Mo ₃ O ₁₂	orthorhombic	-18.1	1073	4
9	Lu ₂ Mo ₃ O ₁₂	orthorhombic	-18.1	1073	4
10	Y ₂ Mo ₃ O ₁₂	orthorhombic	-28.1	1073	4
11	HfMgW ₃ O ₁₂	orthorhombic	-1.9	773	5
12	Fe _{0.2} (HfMg) _{0.9} W ₃ O ₁₂	orthorhombic	-2.0	773	5
13	Fe _{0.6} (HfMg) _{0.7} W ₃ O ₁₂	orthorhombic	-2.5	773	5
14	Fe(HfMg) _{0.5} W ₃ O ₁₂	monoclinic	-3.4	773	5
15	ZrMnMo ₃ O ₁₂	orthorhombic	-8.4	873	6

16	ZrScMo ₂ VO ₁₂	orthorhombic	-6.6	773	7
17	Zr ₂ MoP ₂ O ₁₂	orthorhombic	-13.4	400	8
18	Sc ₂ W ₃ O ₁₂	orthorhombic	-6.6	450	9
19	Lu ₂ W ₃ O ₁₂	orthorhombic	-20.4	900	10
20	Y ₂ W ₃ O ₁₂	orthorhombic	-20.9	1073	11
21	ZrScW ₂ PO ₁₂	orthorhombic	-5.3	1300	12
22	Zr ₂ WP ₂ O ₁₂	orthorhombic	-14.1	298	13
23	Sc _{0.8} (ZrHf) _{0.1} FeMo _{2.8} V _{0.2} O ₁₂	orthorhombic	-0.4	650	13
24	Sc _{0.8} (ZrHf) _{0.2} Fe _{0.8} Mo _{2.6} V _{0.4} O ₁₂	orthorhombic	-0.3	650	13
25	Sc _{0.8} (ZrHf) _{0.3} Fe _{0.6} Mo _{2.4} V _{0.6} O ₁₂	orthorhombic	-2.6	650	13
26	Sc _{0.5} (ZrHf) _{0.5} Fe _{0.5} Mo ₂ VO ₁₂	orthorhombic	-4.0	650	13
27	Zr ₂ MoVPO ₁₂	orthorhombic	-7.0	700	14
28	Fe ₂ Mo ₃ O ₁₂	orthorhombic	-44.5	1023	15
29	Cr ₂ Mo ₃ O ₁₂	orthorhombic	-28.2	1023	15
30	Al ₂ Mo ₃ O ₁₂	orthorhombic	-8.5	1073	15
31	Yb _{1.6} Al _{0.4} (MoO ₄) ₃	orthorhombic	-16.5	840	16
32	Yb _{0.4} Al _{1.6} (MoO ₄) ₃	orthorhombic	17.2	1000	16
33	Yb _{0.2} Al _{1.8} (MoO ₄) ₃	orthorhombic	28.5	950	16
34	Yb _{1.8} Al _{0.2} Mo ₃ O ₁₂	orthorhombic	-27.3	800	16
35	In ₂ Mo ₃ O ₁₂	orthorhombic	-5.6	1033	17
36	HfScMo ₂ VO ₁₂	orthorhombic	-6.3	800	18
37	HfScW ₂ PO ₁₂	orthorhombic	-3.8	1469	19
38	Cr ₂ (WO ₄) ₃	orthorhombic	-21.1	1073	20
39	Dy ₂ (WO ₄) ₃	monoclinic	22.9	1073	21
40	Nd ₂ (WO ₄) ₃	monoclinic	16.6	1073	21
41	In ₂ (WO ₄) ₃	orthorhombic	-9.0	973	22
42	In _{1.9} Sc _{0.1} W ₃ O ₁₂	orthorhombic	-15.9	973	22
43	In _{1.7} Sc _{0.3} W ₃ O ₁₂	orthorhombic	-3.2	973	22
44	In _{1.5} Sc _{0.5} W ₃ O ₁₂	orthorhombic	-3.8	973	22
45	InScW ₃ O ₁₂	orthorhombic	-21.4	973	22
46	Yb ₂ W ₃ O ₁₂	orthorhombic	-19.1	1073	23
47	Er ₂ W ₃ O ₁₂	orthorhombic	-20.2	1073	23
48	HfMg _{0.8} Zn _{0.2} Mo ₃ O ₁₂	orthorhombic	-0.2	673	24
49	HfMg _{0.7} Zn _{0.3} Mo ₃ O ₁₂	orthorhombic	-0.3	673	24
50	HfMg _{0.6} Zn _{0.4} Mo ₃ O ₁₂	orthorhombic	-0.3	673	24
51	HfMg _{0.5} Zn _{0.5} Mo ₃ O ₁₂	orthorhombic	-0.3	840	24
52	HfMgMo _{1.5} W _{1.5} O ₁₂	orthorhombic	-6.2	550	25
53	In(HfMg) _{0.5} Mo ₃ O ₁₂	orthorhombic	-1.2	923	26
54	In _{1.75} Y _{0.25} Mo ₃ O ₁₂	orthorhombic	-11.3	1073	[this work]
55	In _{1.5} Y _{0.5} Mo ₃ O ₁₂	orthorhombic	-10.1	1073	[this work]
56	In _{1.25} Y _{0.75} Mo ₃ O ₁₂	orthorhombic	-13.3	1073	[this work]

57	$\text{InYMo}_3\text{O}_{12}$	orthorhombic	-12.9	1073	[this work]
58	$\text{In}_{0.75}\text{Y}_{1.25}\text{Mo}_3\text{O}_{12}$	orthorhombic	-16.4	1073	[this work]
59	$\text{In}_{0.5}\text{Y}_{1.5}\text{Mo}_3\text{O}_{12}$	orthorhombic	-5.6	1033	[this work]
60	$\text{ZrMg}_{0.7}\text{Al}_{0.3}\text{Mo}_{2.7}\text{V}_{0.3}\text{O}_{12}$	orthorhombic	-7.7	300	27
61	$\text{ZrMg}_{0.4}\text{Al}_{0.6}\text{Mo}_{2.4}\text{V}_{0.6}\text{O}_{12}$	orthorhombic	-9.5	313	27
62	$\text{ZrMg}_{0.3}\text{Al}_{0.7}\text{Mo}_{2.3}\text{V}_{0.7}\text{O}_{12}$	orthorhombic	-11.4	320	27
63	$\text{Y}_{0.25}\text{Nd}_{1.75}(\text{W O}_4)_3$	monoclinic	18.9	800	28
64	$\text{Ho}_2(\text{Mo O}_4)_3$	orthorhombic	-21.8	473	29
65	$\text{Zr}_{0.26}\text{Sc}_{1.74}\text{Mo}_{2.878}\text{V}_{0.122}\text{O}_{12}$	orthorhombic	-5.0	575	30
66	$(\text{Nd}_{1.8}\text{Er}_{0.2})\text{W}_3\text{O}_{12}$	monoclinic	8.3	1073	31
67	$(\text{Nd}_{1.6}\text{Er}_{0.4})\text{W}_3\text{O}_{12}$	monoclinic	7.7	1073	31
68	$(\text{Nd}_{0.5}\text{Er}_{1.5})\text{W}_3\text{O}_{12}$	orthorhombic	-6.3	1073	31
69	$(\text{Nd}_{0.3}\text{Er}_{1.7})\text{W}_3\text{O}_{12}$	orthorhombic	-6.2	1073	31
70	$(\text{Nd}_{0.1}\text{Er}_{1.9})\text{W}_3\text{O}_{12}$	orthorhombic	-6.0	1073	31
71	$\text{Zr}_2\text{P}_2\text{SO}_{12}$	monoclinic	-23.0	373	32
72	$(\text{KMg})_{0.25}\text{Sc}_{1.75}\text{W}_3\text{O}_{12}$	hexagonal	-13.8	700	33
73	$(\text{KMg})_{0.5}\text{Sc}_{1.5}\text{W}_3\text{O}_{12}$	hexagonal	-7.5	700	33
74	$(\text{KMg})_{0.75}\text{Sc}_{1.25}\text{W}_3\text{O}_{12}$	hexagonal	-10.0	700	33
75	$(\text{KMg})\text{ScW}_3\text{O}_{12}$	hexagonal	-14.1	700	33
76	$(\text{KMg})_{1.25}\text{Sc}_{0.75}\text{W}_3\text{O}_{12}$	hexagonal	-13.8	700	33
77	$(\text{KMg})_{1.5}\text{Sc}_{0.5}\text{W}_3\text{O}_{12}$	hexagonal	-5.9	520	33
78	$\text{NaTi}_2\text{P}_3\text{O}_{12}$	trigonal	-0.6	1273	34
79	$\text{NaZr}_2\text{P}_3\text{O}_{12}$	trigonal	-0.4	1273	34
80	Ag_2O	cubic	-31.2	200	35
81	Cu_2O	cubic	-7.2	240	35
82	Au_2O	cubic	-2.0	273	35
83	$\text{CaZr}_4(\text{PO}_4)_6$	trigonal	-0.2	673	36
84	TaVO_5	orthorhombic	-8.9	873	37
85	NbVO_5	orthorhombic	-6.6	873	37
86	$\text{Zr}_{0.5}\text{Hf}_{0.5}\text{V}_2\text{O}_7$	cubic	-2.3	673	38
87	ZrV_2O_7	cubic	-21.0	1023	39
88	HfV_2O_7	cubic	-21.0	300	39
89	ThP_2O_7	cubic	-9.4	1174	40
90	UP_2O_7	cubic	-8.2	1073	40
91	CeP_2O_7	cubic	-5.7	1078	41
92	$\text{Th}_2\text{O}(\text{PO}_4)_2$	orthorhombic	-4.8	873	41
93	$\text{Cu}_2\text{V}_2\text{O}_7$	orthorhombic	-5.3	500	42
94	$\text{Cu}_2\text{V}_2\text{O}_7$	monoclinic	-20.2	673	43
95	$\text{U}_2\text{O}(\text{PO}_4)_2$	orthorhombic	-4.2	873	44
96	NbOPO_4	orthorhombic	-11.0	973	45
97	PbAlBO_4	orthorhombic	18.0	1000	46

98	$\text{K}_2 \text{Th} (\text{P O}_4)_2$	tetragonal	33.6	900	47
99	$\text{Ca}_2 \text{Mn}_{0.35} \text{Ti}_{0.65} \text{O}_4$	tetragonal	17.9	300	48
100	$\text{Ca}_2 \text{Mn}_{0.3} \text{Ti}_{0.7} \text{O}_4$	tetragonal	51.7	400	48
101	$\text{Ca}_{1.6} \text{Sr}_{0.4} \text{Mn O}_4$	tetragonal	30.3	300	48
102	$\text{Ca}_2 \text{Mn O}_4$	tetragonal	38.6	400	48
103	$\text{Ca}_{1.4} \text{Sr}_{0.6} \text{Mn O}_4$	tetragonal	29.9	300	48
104	$\text{Ca}_{1.8} \text{Sr}_{0.2} \text{Mn O}_4$	tetragonal	15.2	300	48
105	$\text{Ca}_2 \text{Mn}_{0.375} \text{Ti}_{0.625} \text{O}_4$	tetragonal	37.0	400	48
106	$\text{Ca}_2 \text{Mn}_{0.575} \text{Ti}_{0.425} \text{O}_4$	tetragonal	37.5	400	48
107	$\text{Ca}_2 \text{GeO}_4$	tetragonal	19.2	400	49
108	$\text{La} (\text{Cr O}_3)$	orthorhombic	22.9	1013	50
109	$\text{Cu}_2 \text{O Cl}_2$	orthorhombic	32.4	723	51
110	$(\text{V}_{0.98} \text{Mo}_{0.02})_2 \text{O}_3$	monoclinic	-3.9	125	52
111	$(\text{V}_{0.97} \text{Mo}_{0.03})_2 \text{O}_3$	monoclinic	-3.9	125	52
112	$(\text{V}_{0.9} \text{Mo}_{0.1})_2 \text{O}_3$	trigonal	16.0	300	52
113	$(\text{V}_{0.8} \text{Mo}_{0.2})_2 \text{O}_3$	trigonal	11.0	300	52
114	$\text{Zr}_{0.5} \text{Sn}_{0.5} \text{Mo}_2 \text{O}_8$	cubic	-6.3	800	53
115	$\text{Zr} (\text{Mo O}_4)_2$	orthorhombic	-3.6	500	54
116	$\text{ZrW}_{1.5} \text{Mo}_{0.5} \text{O}_8$	cubic	-15.3	343	55
117	$\text{ZrW}_{1.8} \text{Mo}_{0.2} \text{O}_8$	cubic	-11.8	403	55
118	$\text{ZrW}_{1.6} \text{Mo}_{0.4} \text{O}_8$	cubic	-9.0	343	55
119	$\text{Cu}_2 \text{Sc}_2 (\text{Ge}_4 \text{O}_{13})$	monoclinic	8.4	293	56
120	$\text{Sr}_2 \text{Mg} (\text{W O}_6)$	tetragonal	21.3	300	57
121	$\text{Zr} (\text{W Mo}) \text{O}_8$	trigonal	69.0	673	58
122	$\text{Zr} (\text{W Mo}) \text{O}_8$	cubic	-4.0	973	59
123	$\text{Cs} (\text{Al Si O}_4)$	orthorhombic	37.9	1098	60
124	$\text{Sn} (\text{Mo}_2 \text{O}_8)$	cubic	30.0	373	61
125	$\text{Sr}_2 (\text{Ir O}_4)$	tetragonal	32.0	1200	62
126	$\text{Zr} (\text{W}_{0.9} \text{Mo}_{0.1})_{1.76} \text{V}_{0.24} \text{O}_{7.88}$	cubic	-11.0	550	63
127	$\text{Sr}_2 \text{Rh O}_4$	tetragonal	43.8	850	64
128	Tc O_2	orthorhombic	24.6	1273	65
129	$\text{Zr} (\text{W O}_4)_2$	cubic	-27.3	693	66
130	Si O_2	monoclinic	-9.1	550	67
131	$\text{Si}_{36} \text{O}_{72}$	orthorhombic	-24.2	560	68
132	$\text{Lu}_5 \text{Ba}_6 \text{B}_9 \text{O}_{27}$	monoclinic	27.7	473	69
133	$\text{Cs}_3 \text{W}_3 \text{P O}_{13}$	orthorhombic	20.6	270	70
134	$\text{Cs}_2 ((\text{Np O}_2)_2 (\text{S O}_4)_3)$	tetragonal	70.1	293	71
135	$\text{Cs}_2 ((\text{NpO}_2)_2 (\text{SeO}_4)_{0.18} (\text{SO}_4)_{2.82})$	tetragonal	56.6	293	71
136	$\text{Cs}_2 ((\text{NpO}_2)_2 (\text{SeO}_4)_{0.55} (\text{SO}_4)_{2.45})$	tetragonal	63.6	293	71
137	$\text{Cs}_2 ((\text{NpO}_2)_2 (\text{SeO}_4)_{1.19} (\text{S O}_4)_{1.81})$	tetragonal	63.0	293	71
138	$\text{Cs}_2 ((\text{Np O}_2)_2 (\text{Se O}_4)_3)$	tetragonal	91.2	293	71
139	$(\text{Er}_{0.25} \text{Dy}_{1.75}) (\text{Mo}_4 \text{O}_{15})$	monoclinic	25.1	773	72
140	$\text{HfW}_2 \text{O}_8$	cubic	-26.4	300	73
141	$\text{HfMo}_2 \text{O}_8$	orthorhombic	-12.0	573	74

142	Zn O	cubic	-5.1	40	75
143	H _{1.90} (Al _{1.90} Si _{190.10} O ₃₈₄)	cubic	-13.8	573	76
144	Si O ₂ (C O ₂) _{0.542}	cubic	-16.7	1173	77
145	Cu Sc O ₂	hexagonal	-4.0	300	78
146	LiAlSiO ₄	trigonal	-6.2	1273	79
147	GeZn ₂ O ₄	trigonal	-2.0	300	80
148	CuZnV ₂ O ₇	monoclinic	-2.3	673	81
149	Cu ₂ P ₂ O ₇	monoclinic	-27.7	373	82
150	Cu _{0.5} Zn _{1.5} P ₂ O ₇	monoclinic	-2.8	225	83
151	CuZnP ₂ O ₇	monoclinic	-4.3	175	83
152	Cu _{1.25} Zn _{0.75} P ₂ O ₇	monoclinic	-6.2	225	83
153	Cu _{1.5} Zn _{0.5} P ₂ O ₇	monoclinic	-12.4	275	83
154	Cu _{1.75} Zn _{0.25} P ₂ O ₇	monoclinic	-15.4	350	83
155	MgH ₂ SO ₅	monoclinic	34.1	293	84
156	FeH ₂ SO ₅	monoclinic	46.6	293	84
157	CoH ₂ SO ₅	monoclinic	33.4	293	84
158	NiH ₂ SO ₅	monoclinic	35.5	293	84
159	(NH ₄) ₂ V ₃ O ₈	tetragonal	82.1	170	85
160	AlPO ₄	hexagonal	-35.1	300	86
161	Ti ₂ O ₃	trigonal	19.0	593	87
162	LiBO ₂	monoclinic	27.0	330	88
163	H ₂ O	hexagonal	-4.0	60	89
164	SrO	cubic	41.2	300	90
165	SrTiO ₃	cubic	28.2	300	90
166	SrZrO ₃	orthorhombic	26.3	300	90
167	TiO ₂	tetragonal	23.7	300	90
168	ZrO ₂	monoclinic	21.2	300	90
169	ZrSiO ₄	tetragonal	12.3	300	90
170	KNbO ₃	tetragonal	15.0	300	90
171	LiAlSi ₂ O ₆	monoclinic	22.2	300	90
172	MgFe ₂ O ₄	cubic	20.5	300	90
173	MgGeO ₃	orthorhombic	22.4	300	90
174	MgO	cubic	32.4	300	90
175	Mg ₂ GeO ₄	cubic	32.1	300	90
176	MnO	cubic	34.5	300	90
177	Mo ₃ Fe ₂ O ₁₂	monoclinic	29.1	300	90
178	NaAlSi ₂ O ₆	monoclinic	24.7	300	90
179	NaAlSi ₃ O ₈	triclinic	26.8	300	90
180	NaCrSi ₂ O ₆	monoclinic	20.4	300	90
181	NaNbO ₃	cubic	33.0	300	90
182	ReO ₃	cubic	-7.7	300	90
183	ScAlO ₃	orthorhombic	27.0	300	90
184	Al ₂ SiO ₅	orthorhombic	13.3	300	90
185	BPO ₄	tetragonal	28.2	300	90

186	BeAl ₂ O ₄	orthorhombic	23.8	300	90
187	BeO	hexagonal	17.0	300	90
188	Be ₂ SiO ₄	trigonal	16.8	300	90
189	CaGeO ₃	orthorhombic	31.1	300	90
190	Ca O ₃ Ti	orthorhombic	75.0	300	90
191	CaO	cubic	37.5	300	90
192	Ca ₃ Al ₂ Si ₃ O ₁₂	cubic	19.2	300	90
193	Ca ₃ Fe ₂ Si ₃ O ₁₂	cubic	20.6	300	90
194	Cr ₂ FeO ₄	cubic	9.9	300	90
195	Cr ₂ MgO ₄	cubic	16.5	300	90
196	FeO	cubic	33.9	300	90
197	FeTiO ₃	trigonal	27.9	300	90
198	Fe ₃ O ₄	cubic	20.6	300	90
199	HfO ₂	monoclinic	15.8	300	90
200	Al ₂ FeO ₄	cubic	15.6	300	90
201	Al ₂ Fe ₃ Si ₃ O ₁₂	cubic	15.8	300	90
202	Al ₂ Mg ₃ Si ₃ O ₁₂	cubic	19.9	300	90
203	AlMn ₃ Si ₃ O ₁₂	cubic	17.2	300	90
204	KF	cubic	95.1	300	90
205	LiF	cubic	106.5	300	90
206	MgF ₂	tetragonal	33.0	300	90
207	NaF	cubic	102.6	300	90
208	NaMgF ₃	orthorhombic	102.0	300	90
209	MnF ₂	tetragonal	20.1	300	90
210	CoF ₂	tetragonal	24.5	300	90
211	NiF ₂	tetragonal	23.4	300	90
212	FeF ₂	tetragonal	33.1	300	90
213	KBr	cubic	117.6	300	90
214	KCl	cubic	114.9	300	90
215	KI	cubic	113.7	300	90
216	LiBr	cubic	146.7	300	90
217	LiCl	cubic	131.1	300	90
218	LiI	cubic	177.0	300	90
219	NaBr	cubic	125.7	300	90
220	NaCl	cubic	121.2	300	90
221	NaI	cubic	135.0	300	90
222	RbBr	cubic	117.0	300	90
223	RbCl	cubic	120.6	300	90
224	RbI	cubic	114.0	300	90
225	Bi ₂ Se ₃	trigonal	41.0	300	90
226	AgCl	cubic	98.7	300	90
227	CuCl	cubic	-10.0	400	90
228	CuBr	cubic	-2.0	320	90
229	AgBr	cubic	102.3	300	90

230	TiC	cubic	22.2	300	90
231	B ₄ C	trigonal	13.5	300	90
232	HgCl	tetragonal	132.8	300	90
233	HgI	tetragonal	115.4	300	90
234	HgI ₂	tetragonal	49.0	300	90
235	SiC	trigonal	14.1	300	90
236	Al ₂ O ₃	trigonal	26.4	300	91
237	Sr ₃ Ir ₂ O ₇	orthorhombic	23.6	300	92
238	Na ₂ Ti ₃ O ₇	monoclinic	21.0	300	93
239	GeMg ₂ O ₄	cubic	9.1	300	94
240	GeCd ₂ O ₄	orthorhombic	10.1	300	94
241	Nb ₁₄ W ₃ O ₄₄	monoclinic	-12.8	433	95
242	SrWO ₄	tetragonal	24.9	620	96
243	BaWO ₄	tetragonal	27.2	620	96
244	PbWO ₄	tetragonal	36.0	620	96
245	CaWO ₄	tetragonal	25.0	620	96
246	CaMoO ₄	tetragonal	27.2	620	96
247	CdMoO ₄	tetragonal	28.8	620	96
248	SrMoO ₄	tetragonal	30.8	300	96
249	PbMoO ₄	tetragonal	37.8	300	96
250	NaIO ₄	tetragonal	131.2	300	96
251	KIO ₄	tetragonal	107.3	300	96
252	RuO ₂	tetragonal	12.4	300	96
253	CrO ₂	tetragonal	22.4	300	96
254	SnO ₂	tetragonal	10.3	300	96
255	PbO ₂	tetragonal	26.1	300	96
256	VO ₂	tetragonal	38.1	300	96
257	GeO ₂	tetragonal	13.9	300	96
258	CaCO ₃	trigonal	25.1	300	96
259	CdCO ₃	trigonal	18.9	300	96
260	MnCO ₃	trigonal	21.8	300	96
261	ZnCO ₃	trigonal	23.5	300	96
262	NaNO ₃	trigonal	113.4	300	96
263	ScBO ₃	trigonal	9.7	300	96
264	CaMgSi ₂ O ₆	monoclinic	28.0	300	97
265	Al	cubic	23.1	300	98
266	Sb	cubic	11.0	300	98
267	Be	cubic	11.3	300	98
268	Cd	hexagonal	30.8	300	98
269	Co	cubic	13.0	300	98
270	Ge	cubic	5.7	300	98
271	Cu	cubic	16.5	300	98
272	Au	cubic	14.2	300	98
273	In	cubic	32.1	300	98

274	Ir	cubic	6.4	300	98
275	Fe	cubic	11.8	300	98
276	Pb	cubic	28.9	300	98
277	Mg	cubic	-0.2	100	98
278	Ni	cubic	13.4	300	98
279	Nb	cubic	7.3	300	98
280	Pd	cubic	11.8	300	98
281	Pt	cubic	8.8	300	98
282	Rh	cubic	8.2	300	98
283	Si	cubic	-0.4	100	98
284	Ag	cubic	18.9	300	98
285	Ta	cubic	6.3	300	98
286	Tl	cubic	29.9	300	98
287	Sn	cubic	22.0	300	98
288	Ti	cubic	8.6	300	98
289	U	cubic	13.9	300	98
290	V	cubic	8.4	300	98
291	Zn	hexagonal	30.2	300	98
292	UP	cubic	8.7	300	98
293	UN	cubic	8.9	300	98
294	Mg ₂ SiO ₄	orthorhombic	9.0	300	99
295	Na Sr ₅ (B O ₃) (Si O ₄) ₂	monoclinic	8.0	300	100
296	BaTi ₄ O ₉	orthorhombic	8.1	300	101
297	Na ₂ Ca ₃ (Si ₆ O ₁₆)	Triclinic	7.5	300	102
298	La ₄ Ti ₂ O ₄ Se ₅	orthorhombic	-0.5	100	103
299	Ba ₂ K ₂ Te ₂ O ₉	hexagonal	6.0	293	104
300	MgSiO ₃	monoclinic	9.0	293	105
301	Al ₂ TiO ₅	orthorhombic	8.0	300	106
302	K Na ₃ (Al ₄ Si ₄ O ₁₆)	hexagonal	49.0	300	107
303	Na Ca ₂ Fe ₅ Si ₈ O ₂₂ (O H) ₂	monoclinic	33.0	300	108
304	Ca ₂ Mg (Si ₂ O ₇)	tetragonal	33.0	300	109
305	Ca ₂ Al ₂ Si O ₇	tetragonal	26.0	300	110
306	Fe ₂ Si O ₄	orthorhombic	31.0	300	111
307	Ca ₃ Mg (Si O ₄) ₂	monoclinic	42.0	300	112
308	Mg ₃ Al ₂ Si ₃ O ₁₂	cubic	26.0	300	113
309	Al ₂ (Si O ₄) (O H) ₂	orthorhombic	25.0	300	114
310	SmFe ₃ (BO ₃) ₄	trigonal	-2.1	400	115
311	Pr ₂ (SO ₄) ₃	monoclinic	15.6	300	116
312	BaZn ₂ Si ₂ O ₇	orthorhombic	0.0	1000	117
313	Ca ₂ RuO ₄	orthorhombic	-48.5	340	118
314	AgCN	trigonal	-14.8	300	119
315	AuCN	hexagonal	-6.9	300	119
316	CuCN	trigonal	-27.9	300	119
317	(Ag _{0.5} Au _{0.5})CN	orthorhombic	-9.0	490	120

318	$(\text{Cu}_{0.5}\text{Au}_{0.5})\text{CN}$	orthorhombic	-13.8	490	120
319	$\text{Zn}(\text{CN})_2$	cubic	-50.7	375	121
320	$\text{Cd}(\text{CN})_2$	cubic	-61.2	375	121
321	$\text{AgB}(\text{CN})_4$	cubic	-40.0	400	122
322	$\text{CuB}(\text{CN})_4$	cubic	-10.0	400	122
323	$\text{ZnNi}(\text{CN})_4$	tetragonal	-27.0	400	123
324	$\text{CuNi}(\text{CN})_4$	tetragonal	-9.7	473	124
325	$\text{CdPt}(\text{CN})_6$	cubic	-30.1	240	125
326	$\text{MnPt}(\text{CN})_6$	cubic	-19.7	300	125
327	$\text{FePt}(\text{CN})_6$	cubic	-12.0	315	125
328	$\text{ZnPt}(\text{CN})_6$	cubic	-10.6	400	125
329	$\text{CoPt}(\text{CN})_6$	cubic	-4.8	350	125
330	$\text{NiPt}(\text{CN})_6$	cubic	-3.1	330	125
331	$\text{CuPt}(\text{CN})_6$	tetragonal	-4.7	400	125
332	$\text{FeFe}(\text{CN})_6$	cubic	-12.8	450	126
333	$\text{GaFe}(\text{CN})_6$	cubic	-12.0	475	127
334	$\text{FeCo}(\text{CN})_6$	cubic	-4.4	300	128
335	$\text{YFe}(\text{CN})_6$	cubic	-33.7	575	129
336	$\text{Y}(\text{Fe}(\text{CN})_6)(\text{H}_2\text{O})_4$	orthorhombic	13.1	300	129
337	$\text{K Y Fe}(\text{CN})_6(\text{H}_2\text{O})_3$	orthorhombic	42.7	300	129
338	$\text{K Y Fe}(\text{CN})_6$	trigonal	20.3	300	129
339	$\text{K La Fe}(\text{CN})_6$	trigonal	50.0	300	130
340	$\text{K La}(\text{Fe}(\text{CN})_6)(\text{H}_2\text{O})_4$	hexagonal	55.8	300	131
341	$\text{La}(\text{Co}(\text{CN})_6)(\text{H}_2\text{O})_5$	hexagonal	44.5	300	131
342	$\text{LaFe}(\text{CN})_6$	hexagonal	-50.0	150	130
343	$\text{SmFe}(\text{CN})_6$	hexagonal	-40.0	525	132
344	$\text{LuFe}(\text{CN})_6$	hexagonal	-30.0	525	132
345	$\text{HoFe}(\text{CN})_6$	hexagonal	-35.0	525	133
346	$\text{LuCo}(\text{CN})_6$	hexagonal	-27.2	500	133
347	$\text{LaCo}(\text{CN})_6$	hexagonal	-44.1	500	133
348	$\text{PrCo}(\text{CN})_6$	hexagonal	-27.2	500	133
349	$\text{SmCo}(\text{CN})_6$	hexagonal	-37.2	500	133
350	$\text{HoCo}(\text{CN})_6$	hexagonal	-30.0	500	133
351	$\text{YCo}(\text{CN})_6$	hexagonal	-31.5	500	133
352	$\text{ScCo}(\text{CN})_6$	cubic	-19.8	600	134
353	$\text{ErCo}(\text{CN})_6$	hexagonal	-27.0	375	135
354	$\text{Er}(\text{Co}(\text{CN})_6)(\text{H}_2\text{O})_4$	orthorhombic	11.0	300	135
355	$\text{Ni}_2\text{W}(\text{CN})_8$	tetragonal	-24.6	260	136
356	$(\text{Ni}(\text{H}_2\text{O})_2)_2(\text{W}(\text{CN})_8)(\text{H}_2\text{O})_4$	tetragonal	35.4	300	136
357	$\text{Co}_3(\text{Co}(\text{CN})_6)_2(\text{H}_2\text{O})_{12}$	cubic	-119.1	298	137
358	$\text{Ni}_3(\text{Co}(\text{CN})_6)_2(\text{H}_2\text{O})_{12}$	cubic	-90.0	298	137
359	$\text{Zn}_3(\text{Co}(\text{CN})_6)_2(\text{H}_2\text{O})_9$	cubic	-89.1	298	137
360	$\text{Mn}_3(\text{Co}(\text{CN})_6)_2(\text{H}_2\text{O})_{12}$	cubic	-87.6	298	137
361	$\text{Cu}_3(\text{Co}(\text{CN})_6)_2(\text{H}_2\text{O})_{12}$	cubic	-60.0	298	137

362	$\text{Fe}_3 (\text{Co} (\text{C N})_6)_2 (\text{H}_2 \text{O})_{12}$	cubic	-58.8	298	137
363	$\text{Zn}_3 (\text{Fe} (\text{C N})_6)_2 (\text{H}_2 \text{O})_{14}$	cubic	-39.6	298	137
364	$\text{Zn}_2 (\text{Fe} (\text{C N})_6) (\text{H}_2 \text{O})_5$	trigonal	129.3	300	137
365	$\text{Cu}_3 (\text{Fe} (\text{C N})_6)_2 (\text{H}_2 \text{O})_{14}$	cubic	-118.8	298	137
366	$\text{Cu}_2 (\text{Fe} (\text{C N})_6)_2 (\text{H}_2 \text{O})_{16}$	cubic	60.3	300	137
367	$\text{Fe}_3 (\text{Fe} (\text{C N})_6)_2 (\text{H}_2 \text{O})_{14}$	cubic	-29.7	298	137
368	$\text{Mn}_3 (\text{Fe} (\text{C N})_6)_2 (\text{H}_2 \text{O})_{14}$	cubic	143.4	300	137
369	$\text{Mn}_2 (\text{Fe} (\text{C N})_6) (\text{H}_2 \text{O})_9$	monoclinic	60.6	300	137
370	$\text{Co}_3 (\text{Fe} (\text{C N})_6)_2 (\text{H}_2 \text{O})_{17}$	cubic	23.7	300	137
371	$\text{Co}_2 (\text{Fe} (\text{C N})_6)_2 (\text{H}_2 \text{O})_{18}$	cubic	58.5	300	137
372	$\text{Ni}_3 (\text{Fe} (\text{C N})_6)_2 (\text{H}_2 \text{O})_{14}$	cubic	17.7	300	137
373	$\text{Ni}_2 (\text{Fe} (\text{C N})_6)_2 (\text{H}_2 \text{O})_{18}$	cubic	59.7	300	137
374	$\text{Hg} (\text{C N})_2$	tetragonal	116.9	300	138
375	$\text{Hg C N} (\text{N O}_3)$	hexagonal	29.2	300	138
376	$\text{Zn} (\text{Au} (\text{C N})_2)_2$	hexagonal	15.1	300	139
377	$\text{Zn} (\text{Ag} (\text{C N})_2)_2 (\text{Ag C N})_{0.57}$	hexagonal	-13.6	375	139
378	$\text{K Mn} (\text{Ag} (\text{C N})_2)_3$	trigonal	61.0	300	140
379	$\text{KNiAu}_3 (\text{CN})_6$	trigonal	62.0	300	141
380	$\text{KCd} (\text{Ag} (\text{CN})_2)_3$	hexagonal	85.0	300	142
381	$\text{KCd} (\text{Au} (\text{CN})_2)_3$	hexagonal	89.7	395	142
382	$(\text{Zn}_{0.8} \text{Cd}_{0.2}) (\text{C N})_2$	cubic	-17.8	375	143
383	$\text{Cd} (\text{N H}_3)_2 (\text{Cd} (\text{C N})_4)$	tetragonal	20.3	300	144
384	$\text{Ni} (\text{C N})_2 (\text{H}_2 \text{O})_{1.5}$	orthorhombic	48.5	300	145
385	$\text{Ag}_3 (\text{Co} (\text{CN})_6)$	trigonal	20.5	300	146
386	CuSCN	hexagonal	19.9	300	147
387	AgC_4N_3	orthorhombic	98.0	300	148
388	KCN	monoclinic	133.0	300	149
389	NaCN	orthorhombic	53.0	300	150
390	$\text{FePd} (\text{CN})_4$	orthorhombic	83.1	500	151
391	NbO_2F	tetragonal	-5.0	500	152
392	TaO_2F	tetragonal	-0.6	400	153
393	ScF_3	cubic	-42.0	110	154
394	ZnF_2	tetragonal	-2.0	63	155
395	CoZrF_6	cubic	10.0	300	156
396	MgZrF_6	cubic	-22.5	300	157
397	CaHfF_6	cubic	-72.0	1000	157
398	$\text{Mg}_{0.5} \text{Zr}_{1.5} \text{F}_7$	cubic	-5.0	125	158
399	LuZrF_7	cubic	-5.0	200	159
400	YbZrF_7	cubic	-6.0	250	160
401	SrZrF_6	cubic	-40.0	300	161
402	CaZrF_6	cubic	-60.0	675	161
403	MnZrF_6	cubic	-13.4	675	156
404	FeZrF_6	cubic	-9.7	675	156
405	NiZrF_6	cubic	54.7	300	156

406	CaNbF ₆	cubic	-65.0	300	162
407	MgNbF ₆	cubic	150.0	300	162
408	NaSbF ₆	cubic	62.0	300	163
409	NaNbF ₆	cubic	-1.0	250	164
410	CaTiF ₆	cubic	-42.0	500	165
411	AlF ₃	trigonal	86.0	300	166
412	(Sc _{0.95} Ga _{0.05})F ₃	cubic	-7.2	900	167
413	(Sc _{0.9} Ga _{0.05} Fe _{0.05})F ₃	cubic	-3.9	900	167
414	(Sc _{0.8} Ga _{0.05} Fe _{0.15})F ₃	cubic	9.9	300	167
415	(Sc _{0.85} Ga _{0.05} Fe _{0.1})F ₃	cubic	6.9	300	167
416	GaN	hexagonal	-0.7	50	168
417	AlN	hexagonal	-0.3	50	168
418	InN	hexagonal	-0.5	50	168
419	CrI ₃	trigonal	-5.6	300	169
420	FeSi ₂	orthorhombic	16.8	300	170
421	GaAs	cubic	-1.7	150	171
422	ZnS	cubic	-3.2	30	172
423	SrAu ₃ Ge	tetragonal	27.5	300	173
424	Cu _{0.66} Zn _{0.34}	cubic	17.5	300	174
425	(Cu _{0.85} Sn _{0.15})	cubic	17.3	300	174
426	Fe _{0.5} Ni _{0.5}	cubic	9.9	300	174
427	Zn(N(CN) ₂) ₂	orthorhombic	20.2	300	175
428	Si(CN ₂) ₂	cubic	-3.7	500	176
429	LiSr ₂ Br ₃ (CN ₂)	cubic	-3.0	30	177
430	MoS ₂	hexagonal	-1.0	200	178
431	YbAl ₃	cubic	-0.3	25	179
432	Cu ₃ N	cubic	-4.0	50	180
433	Li ₃ N	cubic	-20.0	300	181
434	PdZrGe	orthorhombic	-2.0	900	182

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