

AFLOW V 3.1.146

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*          aflow - STEFANO CURTAROLO Duke University 2003-2017
*          High-Throughput ab-initio Computing Project
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LATEST VERSION OF THE FILE: materials.duke.edu/AFLOW/proto.pdf

PROTOTYPES LIB1

STR#	Symmetry	Name	TYPE	PROTO	SG	conc

FCC						
A1,FCC,1,2	fcc/cF4	Fm-3m	A1	Cu	#225	
A2,BCC,58,59	bcc/cI2	Im-3m	A2	W	#229	
A3,HCP,115,117	hcp/hcp2	P6_3/mmc	A3	Mg	#194	
A4,DIA,301,302	cF8	Fd-3m	A4	C (DIA)	#227	books
A5,betaSn,305,306	tI4	I41/amd	A5	betaSn	#141	Navy Database
A6,In,303,304	tI2	I4/mmm	A6	Indium	#139	Navy Database
A7,As,307,308	hR6	R-3m	A7	alphaAs	#166	Kolmogorov
A8						
A9						
A10,Hg,349,350	hR1	R-3m	A10	alphaHg	#166	ICSD

PROTOTYPES BINARY

STR#	Pearson	Symmetry	Name	TYPE	PROTO	SG	notes

FCC							
1,2	fcc/cF4	Fm-3m	A1	Cu		#225	G(pic1N1)
1.cub,2.cub	fcc/cF4	Fm-3m	A1	Cu		#225	G(pic1N1)
3	tP2	P4/mmm	L1_0	AuCu		#123	AB along [001] G(pic1N2,1)
4	hR2	R-3m	L1_1	CuPt		#166	AB along [111] G(pic1N2,2)
5,6	tI6	I4/mmm	beta1/2	AB2		#139	AB2 along [100]z G(pic1N3,2,"
7,8	oI6	Immm	-	MoPt2		#71	AB2 along [011] G(pic1N3,1)
9,10	hP3	P-3m1	alpha1/2	AB2		#164	AB2 along [111]z G(pic1N3,3,"
11,12	oS8	Cmmm	"L1_3"(unofficial)	AB3		#65	"(A.5B.5)B along [111]" M(CdPt3,PdPt
13,15	tP4	P4/mmm	Z1/3	AB3		#123	AB3 along [001]z M(PtTc3) G(
14	tP4	P4/nmm	Z2	A2B2		#129	A2B2 along [001]z G(pic1N4,3,"
16,18	mS8	C2/m	?	AB3		#12	AB3 along [113] G(pic1N4,12)
17	mS8	C2/m	W2	A2B2		#12	A2B2 along [311]z G(pic1N4,7)
19,21	oP4	Pmmm	Y1/3	AB3		#47	AB3 along [011]z G(pic1N4,9)
20	oP4	Pmmm	Y2	A2B2		#47	A2B2 along [011]z M(AgZr) G(pi
22,24	tI8	I4/mmm	DO_22	Al3Ti		#139	AB3 along [201] G(pic1N4,11)
23	tI8	I41/amd	CH "40"	NbP		#141	A2B2 along [201] G(pic1N4,6,N
25,26	cP4	Pm3(bar)m	L1_2	AuCu3		#221	"(A.5B.5)B along [001]" G(pic1N4,1)
27,29	hR4	R-3m	V1/3	AB3		#166	AB3 along [111]z G(pic1N4,10)
28	hR4	R-3m	V2	A2B2		#166	A2B2 along [111]z G(pic1N4,5)
BCC							
58,59	bcc/cI2	Im-3m	A2	W		#229	
58.cub,59.cub	bcc/cI2	Im-3m	A2	W		#229	
60	oS4	Cmmm	D^19_2h	gamma-IrV		#65	AB along [101]
61	cP2	Pm-3m	B2	CsCl		#221	AB along [001]
62,63	hP3	P-3m1	?	AB2		#164	AB2 along [211]
64,65	oF12	Fmmm	?	AB2		#69	AB2 along [011] WARNI FIX NpPd
66,67	tI6	I4/mmm	C11_b	MoSi2		#139	AB2 along [001] WARNI FIX NpPd
68,69	hR4	R-3m	?	AB3		#166	UNDEF
70,72	oS8	Cmmm	?	AB3		#65	UNDEF

71	oS8	Cmma	?	A2B2	#67	UNDEF	
73,75	mP4	P2/m	?	AB3	#10	UNDEF	
74	mP4	P21/m	?	A2B2	#11	UNDEF	
76,78	tP4	P4/mmm	?	AB3	#123	AB3 along [001]z	
77	tP4	P4/nmm	B11	gamma-CuTi	#129	A2B2 along [001]z	
79,81	oI8	Immm	?	AB3	#71	UNDEF	M(MoTi3, Mo3Ti, Nb3Tc, MoTi3, M
80	oI8	Imma	?	A2B2	#74	UNDEF	M(MoTi)
82,83	tP4	P4/mmm	L6_0	CuTi3	#123		
84,86	cF16	Fm-3m	D0_3	AlFe3/BiF3	#225		
85	cF16	Fd-3m	B32	NaTl	#227		
HCP							
115,117	hcp/hcp2	P6_3/mmc	A3	Mg	#194		
116	hP2	P_6m2	B_h	WC	#187		
118,121	oP4	Pmm2	?	AB3	#25	UNDEF	
119	oP4	Pmmn	-	CuTe	#59		
120	oP4	Pmma	B19	AuCd	#51		
123	oI8	C2/m	?	A2B2	#12	UNDEF	
122,124	oI8	Imm2	?	AB3	#44	UNDEF	
125,127	hP4	P-6m2	?	AB3	#187	UNDEF	
126	hP4	P-3m1	?	A2B2	#164	UNDEF	M(RhRu)
128,132	mS12	Cm	?	AB5	#8	UNDEF	
129,134	mS12	C2/m	?	A4B2	#12	BiHf2-134	#12 Hf-Paper
130,137	mS12	C2/m	?	A4B2	#12		
131,135	mS12	C2/m	?	A4B2	#12		
133,140	mS12	Cm	?	A2B4	#8	UNDEF	
136	mS12	Cm	?	A3B3	#8	UNDEF	
138,139	mS12	Cm	?	A3B3	#8	UNDEF	
141,145	oS12	Amm2	?	AB5	#38		
142,147	oS12	Cmcm	?	A4B2	#63	M(RhRu2)	
143,150	oS12	Cmcm	?	A4B2	#63	mistaken for C49, beware	
*144,148	oS12	Cmcm	?	A4B2	#63	NOT RUN	
*146,153	oS12	Amm2	?	A2B4	#38	NOT RUN	
*149,151	oS12	Amm2	?	A3B3	#38	NOT RUN	
*152,157	oS12	Amm2	?	A3B3	#38	NOT RUN	
*154,160	hP6	P-62m	?	AB5	#189	NOT RUN	
*155,158	hP6	P-62m	?	A2B4	#189	NOT RUN	
*156,159	hP6	Cmcm	?	A2B4	#63	NOT RUN	
*161,167	hR6	R32	?	AB5	#155	NOT RUN	
*162,165	hR6	R32	?	A2B4	#155	NOT RUN	
*163,166	hR6	C2/c	?	A2B4	#15	NOT RUN	
*164	hR6	C2	?	A3B3	#5	NOT RUN	
*168,169	hP6	P-6m2	?	AB5	#187	NOT RUN	
*170,175	hP6	P-6m2	?	A2B4	#187	NOT RUN	
*172	mS8	P-6m2	?	A3B3	#187	NOT RUN	
*171,176	hP6	P-3m1	?	A2B4	#164	NOT RUN	
*173,177	hP6	P63/mmc	?	A2B4	#194	NOT RUN	
*174	hP6	P3m1	?	A3B3	#156	NOT RUN	
LAVES AND OMEGAS							
178,179	hP12	P6_3/mm	C14	MgZn2	#194	A4B8 Hex Laves Str	
180,181	oP16	Pnma	D0_11	Fe3C	#62		
182,183	cF24	Fd-3m	C15	Cu2Mg	#227	Cub Laves Phase	
184,185	cP8	Pm3(bar)n	A15	Cr3Si	#223		
186,187	hP8	P6_3/mmc	D0_19	Ni3Sn	#194		
188,189	oS12	Cmcm	C49	ZrSi2	#63		
190,191	hP3	P3m1	omega phase with Z=1/4 !		#164		
192,193	oS8	Cmcm	B33B_f	CrB	#63		
194	oS8	Cmcm		ITl ITl	#63	Pauling	
195	cP8	P2_13	B20	FeSi	#198	Pauling	
196,197	tP4	P4/nmm 02		CdTi	#129	Pauling	
198	oP24	Pbcm		InTh	#57	Pauling	
199	tI16	I4/mcm	B37	SeTl	#140	Pauling	
201	cF8	Fm-3m	B1	NaCl	#225		
202,203	tI10	I4/mmm	D1_3	BaAl4	#139	NEW	
204,205	hP6	P6/mmm	D2_d	CaCu5	#191		

206,207	tI26	I4/mmm	D2_b	ThMn12	#139	
208,209	hP9	P-62m	C22	Fe2P	#189	
210,211	oP12	Pnma	C37	Co2Si	#62	AL1851.cif
212,213	hR19			Th2Zn17	#166	
214,215	cI28	I-43d	D7_3	Th3P4	#220	
216,217	hP3	P6/mmm	C32	AlB2	#191	
218	cF8	F-43m	B3	ZnS	#216	
219	hP4	P63/mc	B4	ZnS	#186	
220,221	hP4	P63/mmc	B8_1	NiAs	#194	
222,223	hP16	P63/mcm	D8_8	Mn5Si3	#193	128601.cif
224,225	hP38	P63/mmc		Th2Ni17	#194	
226,227	cP8	Pm-3n	A15	Cr3Si	#223	
228,229	tP6	P4/nmm	C38	Cu2Sb	#129	
230,231	tI12		C16	CuAl2	#140	
232,233	tI6	I4/mmm	C11_b	MoSi2	#139	
234,235	tI12	I4/mcm	C16	Al2Cu	#140	130617.cif
236,237	hP142	P63/mmc		Cd58Y13	#194	ICSD_102087
****NO 236,237		cI184	Im-3	Cd6Y (Y12Cd68)	#204	130045.cif
****NO 238,239		hp24	P-6m2	Co3V	#187	130340.cif
238,239	hp24	P63/mmc	Pu3Al		#194	Pauling FILE = Co3V
***240,241		P42/mnm	D8_b	CrFe	#136	130307.cif ???? HARD
242,243	oP24	Pmnm02		NbPd3	#59	130379.cif
244,245		P63/mmc	DO_24	Ni3Ti	#194	AL5957.cif
246,247	hP6	P63/mmc		CaIn2	#194	AL5296.cif
248,249	tI12	I41/amd	C_c	ThSi2	#141	AL2272.cif
***250,251	tI6	I4/mmm	C11_a	CaC2	#139	AL1909.cif UNRUNNABLE
252,253	cF24	F-43m	C15_b	AuBe5	#216	AL3669.cif
254,255	tI32	I4/mcm		W5Si3	#140	AL2650.cif
	hP5	P63/mmc	D5_2	La2O3	#194	130882.cif FRAC OCCUP
256	oP8	Pnma	B27	BFe	#62	AL1744.cif
257,258	oP6	Pnmm	C18	FeS2	#58	marcasite AL1657.cif
259,260	hR5	R-3m	C33	Bi2Te3	#166	120146.cif
261,262	cF96	Fd-3m		Ti2Ni	#227	
263,264	tI14	I4/mmm		Ti3Cu4	#139	120654.cif
265,266	tP10			Ti2Cu3	#129	IMPOSSIBLE
267,268	oP6	Pnmm	C18	FeS2	#52	marcasite AL1657.cif
269,270	hP3	P-3m1	C6	CdI2	#164	AL4899.cif
271,272	oS16	Cmcm		Cd3Y	#63	18260.cif
273,274	hP6	P63/mmc	B8_2	Ni2In	#194	28249.cif
273p,274p	hP5	P-6m2	Fe1.5Ge1	partial of Ni2In	#187	Pauling S525640
275,276	hP6	P63/m		Ni2Si	#176	AL5234.cif
277,278	oP8	Pmnm01	DO_a	betaCu3Ti	#59	AL1729.cif
279,280	tI16	I4/mmm	DO_23	Al3Zr	#139	Navy Database
281,282	cP12	Pa-3	C2	FeS2	#205	chris pyrite
283,284	oI12	Imma		GdSi2(1.4)	#74	chris z=(0.0362,0.2138,0.6250)
285,286	tI10	I4/m	D1_a	MoNi4	#87	Navy Database
287,288	tI6	I4/mmm		CuZr2	#139	Pauling file
289,290	cP4	Pm-3m	DO_9	alphaReO3	#221	Navy Database
291,292	tP4	P4/nmm	B10	PbO/PbS	#129	Navy Database
301,302	cF8	Fd-3m	A4	C (DIA)	#227	books
303,304	tI2	I4/mmm	A6	Indium	#139	Navy Database
305,306	tI4	I41/amd	A5	betaSn	#141	Navy Database
307,308	hR6	R-3m	A7	alphaAs	#166	Kolmo
309,310	cF32	Fm-3m		CuPt7	#225	(Ca7Ge) Gus Navy Database
311,312	tI18	I4/mmm		NbNi8	#139	(Pt8Ti) Gus Navy Database
313,314	tI18	I4/mmm		V4Zn5	#139	Navy Database
315,316	hP24	P6_3/mmc	C36	MgNi2	#194	Navy Database
317,318	oS8	Cmca	A11	alphaGa	#64	Navy Database
319,320	cI58	I(-4)3m	A12	alphaMn	#217	Navy Database
321,322	cP20	P4_132	A13	betaMn	#213	Navy Database
323,324	hP3	P3_21-D_3^6	A8	gammaSe	#152	Navy Database
325,326	hP4	P63/mmc	A9	graphite	#194	Navy Database
327,328	tI2	I4/mmm	Aa	alphaPa	#139	Navy Database
329,330	tP30	P4_2/mnm	Ab	betaU	#136	Navy Database/Pauling
331,332	oP8	I4/mmm	Ac	alphaNp	#62	Navy Database/Pauling

333,334	tP4	P4/nmm	Ad	betaNp	#129	Navy Database/Pauling
335,336	hP1	P6/mmm	Af hex	HgSn_{6-10}	#191	Navy Database
337,338	todo	Ag T-50 boron				
339,340	todo	Ah simple cubic				
341,342	todo	Ai betaPo				
343,344	todo	Ak alphaSe				
345,346	todo	Al betaSe				
347,348	todo	A3' alphaLa				
349,350	hR1	R-3m	A10	alphaHg	#166	ICSD A10.A/B
351,352	todo	A14 In2				
353,354	todo	A16 alphaS				
355,356	todo	A17 black P				
357,358	todo	A20 alphaU				
359,360	hP18	P63/mcm		Ga4Ti5	#193	Pauling
361,362	tP20	P42/mnm		Al2Zr3	#136	Pauling
363,364	hP7	P6/mmm		Al3Zr4	#191	Pauling
365,366	oF40	F2dd		Al3Zr2	#43	Pauling
367,368	cF112	Fm-3c		NaZn13	#226	Pauling
369,370	cP7	Pm-3m		CaB6	#221	Pauling
371,372	hP5	P-3m1	D5_19	Al3Ni2	#164	Navy Database
373,374	cI40	I-43m	Ga4Ni(Ga3.62Ni0.97)		#217	Navy Database (vacancies I23, #197)
375,376	oS16	Cmmm		Ga3Pt5	#65	Navy Database
377,378	mS44	C12/m1		Ga9Ni13	#12	Pauling
379,380	cI112	Ia(-3)d		Ga4Ni3	#230	Navy Database
381,382	tI24	I4_1/amd		Ga2Hf	#141	Navy Database
383,384	cF116	Fm-m		C6Mn23	#225	ICSD
385,386	oP44	Pnma		Cu8Hf3	#62	ICSD
387,388	oS68	Cmca		Ni10Zr7	#64	ICSD_240191
389,390	tP3	P4/mmm		Hg2Pt	#123	ICSD_104339
391,392	oP20	Pnma		B4Mg	#62	Pauling
393,394	oI64	Imma		B7Mg	#74	Pauling
395,396	oP16	Pbam		Ge3Rh5	#55	Pauling
397,398	tP14	P4/mbm		In4Ti3	#127	Pauling
399,400	tP34	P4/nmm.O2	V8Sb9	V7.49Sb9	#129	Pauling
401,402	tI160	I-42d		Li3B14	#122	Pauling/Kolmogorov
403,404	tP20	Pa/mbm		LiB3	#127	Pauling/Kolmogorov
405,406	hR4	R-3m		LiB-MS1	#166	Pauling
407,408	hP8	P63/mmc		LiB-MS2	#194	Pauling
411,412	cI58	I-43m		Re24Ti5	#217	Pauling
413,414	mS36	C12/m1		Ni7Zr2	#12	Pauling
415,416	tI40	I4/m		Pt11Zr9	#87	Pauling
417,418	oP20	Pnma		Au4Zr	#62	Pauling
419,420	oI142	Immm		Hf540s17	#71	Pauling
421,422	hP9	P6_222	C40	CrSi2	#180	Pauling
423.424.t0	hP68	P6/m		Ag51Gd14.o3.t0	#175	Pauling
423.424.t1	hP68	P6/m		Ag51Gd14.o3.t1	#175	Pauling
423.424.t2	hP68	P6/m		Ag51Gd14.o3.t2	#175	Pauling
423.424.t3	hP68	P6/m		Ag51Gd14.o2.t3	#175	Pauling
423.424.t4	hP68	P6/m		Ag51Gd14.o2.t4	#175	Pauling
423.424.t5	hP68	P6/m		Ag51Gd14.o2.t5	#175	Pauling
423.424.t6	hP68	P6/m		Ag51Gd14.o2.t6	#175	Pauling
423.424.t7	hP68	P6/m		Ag51Gd14.o1.t7	#175	Pauling
423.424.t8	hP68	P6/m		Ag51Gd14.o1.t8	#175	Pauling
423.424.t9	hP68	P6/m		Ag51Gd14.o1.t9	#175	Pauling
425,426	cF184	Fd-3m		Zn22Zr	#227	Pauling
427,428	oP24	Pnmm		As2Ti	#58	Pauling
429,430	tI84	I4/mmm		Ge10Ho11	#139	Pauling
431,432	hP48	P6_122		Ir3Zr5	#178	Pauling
433,434	oP6	Pnmm		CaCl2	#58	Pauling
435,436	cP5	P-43m		CFe4	#215	Pauling
437,438	mS28	C12/c1		C2Mn5	#15	Pauling
439,440	oP40	Pnma		C3Mn7	#62	Pauling
441,442	hP20	P6_3mc		Fe3Th7	#186	Pauling
443,444	hR24	R-3cr		F3Fe	#167	Pauling

445,446	hR24	P321		F3Fe	#150	Pauling
447,448	mP4	P12_1/m1		NiTi	#11	Pauling
449,450	cP6	Pn-3m	C3	Ag20	#224	ICSD_281041 Cuprite
451,452	hP9	P-3	Bb	etaAg2Zn	#147	Navy Database
453,454	mS16	C2/m	DO_15	AlCl3	#12	ICSD_39566
455,456	hR8	R32	DO_14	AlF3	#155	ICSD_30274
457,458	hR10	R-3c	D5_1	alphaAl203	#167	ICSD_75479 Corundum
459,460	cI26	Im-3		Al12W	#204	ICSD_58207
461,462	oP12	P212121		Ag2Se	#19	ICSD_15213 Naumannite
463,464	hR26	R-3		AlPd	#148	ICSD_58112
465,466	cP16	Pa-3	SC16	AlSb	#205	ICSD_41994
467,468	cI52	I-43m	gammaBrass	Cu5Zn8	#217	Pauling
469,470	hR36	R-3m h		BaPb3	#166	Pauling
471,472	hP8	Cmcm		Hf3Sc*-h321	#63	Hf-Paper
473,474	hP6	P-62m		Hf5Sc-h51	#189	Hf-Paper
475,476	mS12	C2/m		BiHf2-134	#12	Hf-Paper
477,478	tP6	P4/mmm		Hf5Pb-f63	#123	Hf-Paper
479,480	oS12	Cmmm		HfPd5	#65	Hf-Paper
481,482	hR276	R-3ch		Re25Zr21	#167.2	Pauling
483,484	tP6	P4/mmm	B11_3		#123	Mike Mehl bcc_AAABBB^[001]
485,486	tP6	P4mm	B11_3'		#99	Mike Mehl bcc_AABBBAB^[001]
487,488	tP6	P4/mmm	Z3		#123	Mike Mehl fcc_AAABBB^[001]
489,490	tP6	P4mm	Z3'		#99	Mike Mehl fcc_AABBBAB^[001]
491,492	oP102	Pmn2_1	Al13Co4		#31	Pauling - Grin J_Al_Comp_206_243_1994
493,494	ms102	C1m1	Al12.13Co4	eta	#8	Pauling - Hurd Acta Cryst 15 441 1962
495,496	hP28	P6_3/mmc	Al5Co2	D8_11	#194	Pauling
497,498	mp22	P12_1/c1	Al9Co2		#14	Pauling
499,500	tP10	P-42_1c		Pd4Se	#114	Pauling
501,502	cF1192	Fd(-3)m		NaCd2	#227	Samson, Nature 195, 259 (1962)
503,504	hP10	P6_3/m		Er3Ru2	#176	Pauling
505,506	oP40	Pnma		Pt3Sr7	#62	Pauling
507,508	cF120	Fm-3m		Ir4Sc11	#225	Pauling
509,510	oP276	Pnna		Ru25Y44	#52	Pauling
511,512	cP252	P4_132		RuZn6	#213	Pauling
513,514	mP4	P21/m	B19'	NbRu-Beta''	#11	Eur.Phys.J.B 72 575(2009)
515,516	cF96	Fd-3m		delta(CdNi)	#227.2	Pauling
517,518	hP3	P-3m1		Cd2Ce	#164	Pauling
519,520	hP3	P6/mmm		Hg2U	#191	Pauling
521,522	hP9	P-62m		InMg2	#189	Pauling
523,524	oS16	Cmcm		Cd3Er	#63	Pauling
525,526	hP8	P6_3/mmc		CdMg3	#194	Pauling
527,528	hP24	P6_3/mmc		CeNi3	#194	Pauling
529,530	oP32	Pnma		CoSc3	#62	Pauling
531,532	tP4	P4/mmm		Pb3Sr	#123	Pauling
533,534	hR36	R-3mh		PuNi3	#166	Pauling
535,536	oP16	Pnma		YZn3	#62	Pauling
537,538	hR4	R-3m		Co2Y2*	#166	hcp-paper definition
539,540	mS12	C2/m		Sc2Zr*	#12	hcp-paper definition
541,542	oI8	Immm		Mo3Ti*-81	#71	hcp-paper/monster
543,544	oI8	Imma		MoTi*-80	#74	hcp-paper/monster
545,546	hR3	P-3m1		ReTi2*-81	#164	hcp-paper
547,548	tI6	I4/mmm		Hf2Tl*-6	#139	hf-paper
549,550	oF12	Fmmm		Be2Zn*-65	#69	hcp-paper
551,552	oI8	Imm2		Re3Ru*-124	#44	hcp-paper
553,554	hP24	P63cm	DO_21	Cu2.82P	#185	Pauling
555,556	oP108	Pnma		Mg2Au	#62	Pauling
557,558	cF16	Fm-3m		BiF3	#225	Pearson's crystal data
559,560	cI58	I-43m		Al12Mg17	#217	Pauling
561,562	oS160	Cmcm		MgAu3-x	#63	Pauling
563,564	oS64	Cmcm		MgAu3+x	#63	Pauling
565,566	oF48	Fddd		Mg2Cu	#70	Pauling
567,568	hP18	P-62c		Mg2Ga	#190	Pauling
569,570	Pbam	Pbam		MgGa2	#55	Pauling
571,572	oI28	Ibam		Mg5Ga2	#72	Pauling
573,574	tI28	I4/mmm		Mg2Ga5	#139	Pauling

575,576	tI32	I41/a		MgGa	#88	Pauling
577,578	hR72/24	R32		Mg3Hg	#155	Pauling
579,580	hR48/16	R-3m		Mg3In	#166	Pauling
581,582	cF408	F-43m		Mg44Rh7	#216	Pauling
583,584	cF12	Fm-3m		CaF2	#225	Pauling
585,586	hP8	P63/mmc	DO_18	Al3Ir	#194	Pauling
587,588	cP116	Fm-3m		Mn23Th6	#225	Pauling
589,590	cP39	Pm-3		Mg2Zn11	#200	Pauling
591,592	mS110	C2/m		Mg4Zn7	#12	Pauling
593,594	cP20	P4_132		Mg3Ru2	#213	Pauling
595,596	oS12	Cmcm		Au2V	#63	Pauling
597,598	hP94	P63/mmc		Sr9Mg38	#194	Pauling
600.ABCDE	tP30	P4_2/mnm	sigma	CrFe	#136	Pauling
600.XXXXX where X can be A,B (a total of 32 poscars)						
611,612	cP140	Pm-3		Rh13Sc57	#200	Pauling
613,614	hR13	Imm2		Fe7W6	#166	Pauling
615,616	oP24	Pbca		AuSn2	#61	Pauling
617,618	mS12	C2./m		Bi2Pd	#12	Pauling
619,620	mS28	C2./m		Bi2Pd5	#12	Pauling
621,622	oP16	Pnma		Bi3Ni	#62	Pauling
623,624	oP32	Pnma		Bi3Y5	#62	Pauling
625,626	cI120	Ia-3d		Bi4Rh	#230	Pauling
627,628	hR48	R-3m		BiMn3	#166	Pauling
629,630	oP16	Pmma		BiPd3	#51	Pauling
631,632	tI12	I4/mmm		BiTi2	#139	Pauling
633,634	mP12	P2_{1}./c		CoSb2	#14	Pauling
635,636	hR78	R3m		Cu7Hg6	#160	Pearson (Gamma-Brass Cu5Zn8 Modified)
637,638	oI12	Imma		Hg2K	#74	Pauling
639,640	cI52	I-43m		Ir2Zn11	#217	Pauling files (Gamma-Brass Cu5Zn8 Modified)
641,642	tI32	I-4	DO_e	Ni3P	#82	Pauling
643.AB/BA	aP32	P-1		KP15	#2	Pauling
644.AB/BA	tI116	I4_1/a		Pu28Zr	#88	Pauling
645.AB/BA	cF52	Fm-3m		Bi2U	#225	Pauling
646.AB/BA	oS68	Cmcm		TiZn16	#63	Pauling
647.AB/BA	tI140	I4/mcm		Rh2Y3	#140	Pauling
648.AB/BA	tP32	P4/ncc		Rh3Pu5	#130	Pauling
649.AB/BA	tI32	I-42m		alpha-SV3	#121	Pauling
650.AB	oP12	Pmma		IrTa	#51	Pauling
651.AB/BA	oP36	Pnma		Ge4Sm5	#62	Pauling
652.AB/BA	oP12	Pnma		Cl2Pb	#62	Pauling
653.AB/BA	mP16	P12_1		NbPt3	#11	Pauling
654.AB/BA	cI10	Im-3m		Hg4Pt	#229	Pauling
655.AB/BA	hR14	R-3		Pd4Pu3	#148	Pauling
656.AB/BA	hR15	R-3		Er3Ni2	#148	Pauling
657.AB/BA	oI6	Immm		Pd2Ti	#71	Pauling
658.AB/BA	tP8	P4/mmm		Pd5Ti3	#123	Pauling
659.AB/BA	oS20	Cmcm		Pd3Ti2	#63	Pauling
660.AB/BA	tP14	P4/mbm		Hg5Mn2	#127	Pauling
661.AB/BA	oS32	Cmcm		Pu3Pd5	#63	Pauling
662.AB/BA	oS12	Cmmm		Ga2Zr	#65	G. Ghosh and M.Asta, Acta Mat. 53, 322
663.AB/BA	mP30	P21/c		FeP4_mP30	#14	Pauling
664.AB/BA	mS40	C2/C		FeP4_mS40	#15	Pauling
665.AB/BA	tP16	P4/2mmm		In3Ir	#136	Pauling
666.AB/BA	mS44	C2/m		Fe6Ge5	#12	Pauling
667.AB/BA	mS42	C2/m		Fe3Ga4	#12	Pauling
668.AB/BA	oS28	Cmcm		Al6Mn	#63	Pauling
669.AB	oP8	Pnma		AsFe	#62	Pauling
670.AB/BA	hP6	P6/mmm	B35	CoSn	#191	Pauling
671.AB/BA	cI32	Im-3	DO_2	As3Co	#204	Pauling
672.AB/BA	cI32	Im-3m			#229	Mike - 16 atom scell fcc, A15B1
673.AB/BA	cP16	Pm-3m			#221	Mike - 16 atom scell bcc, A15B1
674.A/B	hP3	P6/mmm			#191	Mike - omega phase (C32) in pure form
675.A/B	cP8	Pm-3n			#223	Mike - A15 phase in pure form
676.AB/BA	hP22	P6/mmc	Fe6.5Ge4-ideal (Fe14Ge8)		#194	Pauling
676p.AB/BA	oS42	Amm2	Fe6.5Ge4-part (Fe13Ge8)		#38	Pauling

677.AB/BA	hR26	R3m		Al8Cr5	#160.2	ICSD_606753	
678.AB/BA	tI24	I4mm		Co5Ge7	#107	ICSD_43386	
679.AB/BA	cP5	Pm-3m	E2_1		#221	NAVY	
680.AB/BA	tP12	P4/mmm		beta-NW2	#123	NAVY (Hagg, sort of)	
681.AB/BA	hR3	R3m		alpha-MoS2	#160	NAVY	
682.AB/BA	hR13	R-3m	D8_5r		#166	NAVY	
683.AB/BA	cI50	Im-3m		Na13Cl12v7	#229	NAVY	
684.A/B	cP8	P2_13		alpha-N2	#198	NAVY	
685.A/B	cP8	Pa-3		alpha-N2p	#205	NAVY	
686.A/B	hP4	P6_3/mmc		beta-N2	#194	NAVY	
687.A/B	hR16	R-3c		epsilon-N2	#167	NAVY	
688.A/B	tP4	P4_2/mnm		gamma-N2	#136	NAVY	
689.AB/BA	hP6	P6_3/mmc		WN2_194af	#194	NAVY	
690.AB/BA	mP12	P2_1/c		Ag2Te	#14	NAVY	
691.AB/BA	cF12	Fm-3m	C1		#225	NAVY	
692.AB/BA	hR3	R-3m	C19		#166	NAVY	
693.AB/BA	tP6	P4_2/mnm	C4		#136	NAVY	
694.AB/BA	hP6	P6_3/mmc	C7		#194	NAVY	
695.AB/BA	hP3	P-6m2		WN2_187fg	#187	NAVY	
696.AB/BA	hP6	P6_3/mmc		WN2_194de	#194	NAVY	
697.AB/BA	tP10	P4_2/mmc		Hagg_N4W6	#131	NAVY	
698.AB/BA	oP16	Pnma		MoO3	#62	NAVY	
699.AB/BA	hP12	P6/mmm		O3W	#191	NAVY	
700.AB/BA	oP16	Pnma		P3Tc	#62	NAVY	
701.AB/BA	hP5	P-3m1		WN4_164ad	#164	NAVY	
702.AB/BA	hP20	P6_3/mmc		B4W	#194	NAVY	
703.AB/BA	oP40	Pbca		P4Re	#61	NAVY	
704.AB/BA	hP14	P6_3/mmc	B8_1v2		#194	NAVY	
705.AB/BA	oS28	Cmca	B8_1v2p		#64	NAVY	
706.AB/BA	oS14	Cmmm		Na4Cl3v1	#65	NAVY	
707.AB/BA	cP7	P-43m		C4W3	#215	NAVY	
708.AB/BA	cP7	Pm-3m		S3U4	#221	NAVY	
709.AB/BA	mS14	C2/m		O5Nb2	#12	NAVY	
710.AB/BA	hP13	P-3m1	B8_1v3		#164	NAVY	
711.AB/BA	cF52	Fm-3m		Na7Cl6_v3	#225	NAVY	
712.AB/BA	cF60	Fm-3m		Na7Cl8v1	#225	NAVY	
713.AB/BA	hP15	P-3m1	B8_1v1		#164	NAVY	
714.AB/BA	hP15	P-6m2	B8_1v1p		#187	NAVY	
715.AB/BA	tP2	P4/mmm		Na1Cl1v2	#123	NAVY	
716.AB/BA	tP6	P4/mmm		Na3Cl3v2	#123	NAVY	
717.AB/BA	hP14	P3m1	B8_1v2pp		#156	NAVY	
718.AB/BA	hR6	R3m	B3v2		#160	NAVY	
719.AB/BA	cF56	F-43m		Na7Cl7v2	#216	NAVY	
720.AB/BA	cF8	Fm-3m	B1		#225	NAVY	
721.AB/BA	hP6	P-62m		NTa	#189	NAVY	
722.AB/BA	cP6	Pm-3m		NbO	#221	NAVY	
723.AB/BA	hP16	P6_3mc		NbS	#186	NAVY	
724.AB/BA	tP3	P4/mmm		Hagg_NW2	#123	NAVY	
725.AB/BA	tI12	I4_1/amd		Mo2N	#141	NAVY	
726.AB/BA	hP9	P-31m		NV2	#162	NAVY	
727.AB/BA	hP9	P-3m1		NW2_Pearson	#164	NAVY	
728.A/B	cP8	Pm-3n	beta-W		#223	NAVY	
729.AB/BA	oP76	Pnma		Ge8Mn11	#62	Pauling	
730.AB/BA	hP48	P-3c1		NaTe3	#165	ICSD_61355	
731.AB/BA	oP48	Pbcn		NaTe	#60	ICSD_61382	
732.AB/BA	mP40	P121/c1		Sb3Sr2	#60	ICSD_32033	
733.AB/BA	mS16	C12/m1		SrAs3	#12	ICSD_41831	
734.AB/BA	tI12	I4/mmm		La2Sb	#139	ICSD_10442	
735.AB/BA	oP32	Pnma		Ga5Tm3	#62	ICSD_104009	
**** BORIDES PROJECT							
1000.AB/BA	cP7	Pm-3m		B6Si1	#221	ICSD_20240	binary_boride_ICSD_frequ
1001.AB/BA	cF52	Fm-3m		B12Y1	#225	ICSD_23860	binary_boride_ICSD_frequ
1002.AB/BA	tP20	P4/mbm		B4La1	#127	ICSD_2360	binary_boride_ICSD_frequ
1003.AB/BA	hP3	P6/mmm		B2Nb1	#191	ICSD_30328	binary_boride_ICSD_frequ
1004.AB/BA	hP3	P6/mmm		B2Pu1	#191	ICSD_43660	binary_boride_ICSD_frequ

1005.AB/BA	tI12	I4/mcm	B1Mo2	#140	ICSD_24278	binary_boride_ICSD_frequ
1006.AB/BA	oS8	Cmcm	B1Ni1	#63	ICSD_26937	binary_boride_ICSD_frequ
1007.AB/BA	hP3	P6/mmm	B2Mg1	#191	ICSD_26675	binary_boride_ICSD_frequ
1008.AB	cF8	F-43m	As1B1	#216	ICSD_43871	binary_boride_ICSD_frequ
1009.AB/BA	oI14	Immm	B4Cr3	#71	ICSD_33704	binary_boride_ICSD_frequ
1010.AB	cF8	Fm-3m	B1Pu1	#225	ICSD_43661	binary_boride_ICSD_frequ
1011.AB/BA	tP10	P4/mbm	B2V3	#127	ICSD_88317	binary_boride_ICSD_frequ
1012.AB/BA	oP8	Pnma	B1Ti1	#62	ICSD_24701	binary_boride_ICSD_frequ
1013.AB/BA	hP20	P6_{3}m	B3Ru7	#186	ICSD_44343	binary_boride_ICSD_frequ
1014.AB/BA	oS20	Cmcm	B3V2	#63	ICSD_79258	binary_boride_ICSD_frequ
1015.AB/BA	cF116	Fm-3m	B6Fe23	#225	ICSD_54786	binary_boride_ICSD_frequ
1016.AB/BA	hP3	P6/mmm	Ag1B2	#191	ICSD_43821	binary_boride_ICSD_frequ
1017.AB/BA	oP8	Pnma	B1Co1	#62	ICSD_612863	binary_boride_ICSD_frequ
1018.AB/BA	tI12	I4/mcm	B1Co2	#140	ICSD_42531	binary_boride_ICSD_frequ
1019.AB/BA	oP16	Pnma	B1Co3	#62	ICSD_44339	binary_boride_ICSD_frequ
1020.AB/BA	tI16	I4_{1}/amd	B1Mo1	#141	ICSD_24280	binary_boride_ICSD_frequ
1021.AB/BA	oS16	Cmcm	B1Re3	#63	ICSD_43662	binary_boride_ICSD_frequ
1022.AB	hP2	P-6m2	B1Tc1	#187	ICSD_168895	binary_boride_ICSD_frequ
1023.AB/BA	hP6	P6_{3}/mmc	B2Re1	#194	ICSD_23871	binary_boride_ICSD_frequ
1024.AB/BA	oP6	Pmnm	B2Ru1	#59	ICSD_31871	binary_boride_ICSD_frequ
1025.AB/BA	hP10	P6_{3}/mmc	B3Ru2	#194	ICSD_23715	binary_boride_ICSD_frequ
1026.AB/BA	oP10	Pnmm	B4Cr1	#58	ICSD_186851	binary_boride_ICSD_frequ
1027.AB/BA	oI10	C2/m	B4Mn1	#12	ICSD_15079	binary_boride_ICSD_frequ
1028.AB/BA	hR7	R-3m	B5W2	#166	ICSD_20326	binary_boride_ICSD_frequ
1029.AB/BA	cF48	F-43m	B1Li1	#216	ICSD_164841	binary_boride_ICSD_frequ
1030.AB/BA	hR12	R3m	B1Li1	#160	ICSD_164842	binary_boride_ICSD_frequ
1031.AB/BA	cF48	F-43m	B1Li1	#216	ICSD_164843	binary_boride_ICSD_frequ
1032.AB/BA	tI24	I-4m2	B1Li1	#119	ICSD_164844	binary_boride_ICSD_frequ
1033.AB/BA	tI24	I-4m2	B1Li1	#119	ICSD_164845	binary_boride_ICSD_frequ
1034.AB/BA	tI26	I4/mmm	B12Sc1	#139	ICSD_615424	binary_boride_ICSD_frequ
1035.AB/BA	hR15	R-3m	B12Si3	#166	ICSD_615435	binary_boride_ICSD_frequ
1036.AB/BA	cF12	Fm-3m	B1Be2	#225	ICSD_20384	binary_boride_ICSD_frequ
1037.AB/BA	oP16	Pnma	B1Co3	#62	ICSD_603543	binary_boride_ICSD_frequ
1038.AB/BA	oP16	Pnma	B1Co3	#62	ICSD_612862	binary_boride_ICSD_frequ
1039.AB/BA	oF48	Fddd	B1Cr2	#70	ICSD_188474	binary_boride_ICSD_frequ
1040.AB/BA	tP3	I4/mcm	B1Fe2	#140	ICSD_160789	binary_boride_ICSD_frequ
1041.AB/BA	tI12	I-42m	B1Fe2	#121	ICSD_16809	binary_boride_ICSD_frequ
1042.AB/BA	hP8	P6_{3}22	B1Fe3	#182	ICSD_184958	binary_boride_ICSD_frequ
1043.AB/BA	oP8	Pnma	B1Li1	#62	ICSD_153291	binary_boride_ICSD_frequ
1044.AB/BA	oP16	Pnma	B1Ni3	#62	ICSD_24306	binary_boride_ICSD_frequ
1045.AB/BA	oP6	Pnmm	B1Pd2	#58	ICSD_10487	binary_boride_ICSD_frequ
1046.AB/BA	oP16	Pnma	B1Pd3	#62	ICSD_43514	binary_boride_ICSD_frequ
1047.AB/BA	hP4	P6_{3}/mmc	B1Pt1	#194	ICSD_24363	binary_boride_ICSD_frequ
1048.AB/BA	hP4	P6_{3}/mmc	B1Pt1	#194	ICSD_615210	binary_boride_ICSD_frequ
1049.AB/BA	hP6	P6_{3}/mmc	B1Pt2	#194	ICSD_615207	binary_boride_ICSD_frequ
1050.AB/BA	oS8	Cmcm	B1Rh1	#63	ICSD_150732	binary_boride_ICSD_frequ
1051.AB/BA	oP12	Pnma	B1Rh2	#62	ICSD_24699	binary_boride_ICSD_frequ
1052.AB/BA	hP4	P6_{3}/mmc	B1Tc1	#194	ICSD_168897	binary_boride_ICSD_frequ
1053.AB/BA	hP4	P6_{3}/mmc	B1Tc1	#194	ICSD_168898	binary_boride_ICSD_frequ
1054.AB	cP2	Pm-3m	B1Tc1	#221	ICSD_168900	binary_boride_ICSD_frequ
1055.AB/BA	tI12	I4/mcm	B1Ti2	#140	ICSD_189385	binary_boride_ICSD_frequ
1056.AB/BA	oS46	Cmmm	B20Na3	#65	ICSD_407159	binary_boride_ICSD_frequ
1057.AB/BA	oP12	Pnma	B2Fe1	#62	ICSD_425310	binary_boride_ICSD_frequ
1058.AB/BA	hR4	R-3m	B2Li2	#166	Kolmogorov-Curtarolo LiB	binary_bor
1059.AB/BA	hP8	P6_{3}/mmc	B2Li2	#194	Kolmogorov-Curtarolo LiB	binary_bor
1060.AB/BA	mS28	C2/c	B2Pd5	#15	ICSD_43513	binary_boride_ICSD_frequ
1061.AB/BA	cF24	Fd-3m	B2Sc1	#227	ICSD_106903	binary_boride_ICSD_frequ
1062.AB/BA	oS6	P6/mmm	B2Tm1	#191	ICSD_44598	binary_boride_ICSD_frequ
1063.AB/BA	hP12	P6_{3}/mmc	B2W1	#194	ICSD_23716	binary_boride_ICSD_frequ
1064.AB/BA	tI32	I4/mcm	B3Cr5	#140	ICSD_41932	binary_boride_ICSD_frequ
1065.AB/BA	hR8	R-3m	B3Mo1	#166	ICSD_167734	binary_boride_ICSD_frequ
1066.AB/BA	oP28	Pnma	B3Ni4	#62	ICSD_24307	binary_boride_ICSD_frequ
1067.AB/BA	mS28	C2/c	B3Ni4	#15	ICSD_24308	binary_boride_ICSD_frequ
1068.AB/BA	hP8	P6_{3}/mmc	B3Re1	#194	ICSD_24361	binary_boride_ICSD_frequ
1069.AB/BA	oS20	P6_{3}/mmc	B3Ru2	#194	ICSD_108082	binary_boride_ICSD_frequ

1070.AB/BA	oI64	Imma		B3Si1	#74	ICSD_412621	binary_boride_ICSD_frequ
1071.AB/BA	oI14	Immm		B4Mn3	#71	ICSD_44446	binary_boride_ICSD_frequ
1072.AB/BA	tP16	P4_{2}/mmc		B4Mn4	#131	ICSD_74985	binary_boride_ICSD_frequ
1073.AB/BA	hP10	P6_{3}/mmc		B4Mo1	#194	ICSD_167735	binary_boride_ICSD_frequ
1074.AB/BA	hP20	P6_{3}/mmc		B4Mo1	#194	ICSD_182095	binary_boride_ICSD_frequ
1075.AB/BA	hR6	R-3m		B4Mo2	#166	ICSD_39554	binary_boride_ICSD_frequ
1076.AB/BA	hP18	P6_{3}/mmc		B4Rh5	#194	ICSD_86395	binary_boride_ICSD_frequ
1077.AB/BA	hP20	P6_{3}/mmc		B4W1	#194	ICSD_43193	binary_boride_ICSD_frequ
1078.AB/BA	tP20	P4/mbm		B4W1	#127	ICSD_615683	binary_boride_ICSD_frequ
1079.AB/BA	mP28	P2_{1}/c		B5Gd2	#14	ICSD_62067	binary_boride_ICSD_frequ
1080.AB/BA	hP14	P6_{3}/mmc		B5Mo2	#194	ICSD_167733	binary_boride_ICSD_frequ
1081.AB/BA	mS14	C2/m		B5W2	#12	ICSD_20326	binary_boride_ICSD_frequ
1082.AB/BA	hP14	P6_{3}/mmc		B5W2	#194	ICSD_615696	binary_boride_ICSD_frequ
1083.AB/BA	oS22	Cmmm		B6Ta5	#65	ICSD_68538	binary_boride_ICSD_frequ
1084.AB/BA	oP38	Pbam		B8Ru11	#55	ICSD_43663	binary_boride_ICSD_frequ
1085.AB/BA	hP20	P6_{3}cm		B9Li1	#185	ICSD_164625	binary_boride_ICSD_frequ

**** CARBIDE PROJECT

001.AA	fcc/cF4	Fm-3m	A1	Cu	#225	from gndstate	
001.BB	fcc/cF4	Fm-3m	A1	Cu	#225	from gndstate	
058.AA	bcc/cI2	Im-3m	A2	W	#229	from gndstate	
058.BB	bcc/cI2	Im-3m	A2	W	#229	from gndstate	
115.AA	hcp/hcp	P6_3/mmc	A3	Mg	#194	from gndstate	
115.BB	hcp/hcp	P6_3/mmc	A3	Mg	#194	from gndstate	
201.AB	cF8	Fm-3m	B1	NaCl	#225	from gndstate	
061.AB	cP2	Pm-3m	B2	CsCl	#221	from gndstate	
218.AB	cF8	F-43m	B3	ZnS	#216	from gndstate	
219.AB	hP4	P63/mc	B4	ZnS	#186	from gndstate	
116.AB	hP2	P_6m2	B_h	WC	#187	from gndstate	
301.AA	cF8	Fd-3m	A4	C (DIA)	#227	BOOK	
301.BB	cF8	Fd-3m	A4	C (DIA)	#227	BOOK	
325.AA	hP4	P63/mmc	A9	C (GRA)	#194	BOOK	
325.BB	hP4	P63/mmc	A9	C (GRA)	#194	BOOK	
1200.AB	cF8	Fm-3m		C1Ti1	#225	ICSD_1546	binary_carbide_ICSD_frequ
1201.AB	cF8	F-43m		C1Si1	#216	ICSD_24217	binary_carbide_ICSD_frequ
1202.AB/BA	tI6	I4/mmm		C2U1	#139	ICSD_14330	binary_carbide_ICSD_frequ
1203.AB/BA	cI40	I-43d		C3Pr2	#220	ICSD_2444	binary_carbide_ICSD_frequ
1204.AB	hP2	P-6m2		C1W1	#187	ICSD_15406	binary_carbide_ICSD_frequ
1205.AB	cP2	Pm-3m		C1Sc1	#221	ICSD_181048	binary_carbide_ICSD_frequ
1206.AB/BA	hR3	R-3m		C1Y2	#166	ICSD_22283	binary_carbide_ICSD_frequ
1207.AB/BA	tP70	P4/mnc		C4Sc3	#128	ICSD_71145	binary_carbide_ICSD_frequ
1208.AB/BA	tP68	P-42_{1}c		C19Er15	#114	ICSD_76817	binary_carbide_ICSD_frequ
1209.AB/BA	oP16	Pnma		C1Fe3	#62	ICSD_16593	binary_carbide_ICSD_frequ
1210.AB/BA	hP3	P-3m1		C1Nb2	#164	ICSD_43670	binary_carbide_ICSD_frequ
1211.AB/BA	mS12	C2/c		C2Ca1	#15	ICSD_54184	binary_carbide_ICSD_frequ
1212.AB/BA	cP12	Pa-3		C2Th1	#205	ICSD_77470	binary_carbide_ICSD_frequ
1213.AB/BA	oP18	Pbam		C5Y4	#55	ICSD_84869	binary_carbide_ICSD_frequ
1214.AB/BA	cI132	Im-3		C6OK6	#204	ICSD_66879	binary_carbide_ICSD_frequ
1215.AB/BA	cF116	Fm-3m		C6Cr23	#225	ICSD_62667	binary_carbide_ICSD_frequ
1216.AB/BA	mP22	P2_{1}/c		C7Ho4	#14	ICSD_83381	binary_carbide_ICSD_frequ
1217.AB/BA	cF12	Fm-3m		Be2C1	#225	ICSD_41567	binary_carbide_ICSD_frequ
1218.AB/BA	oP6	Pnmm		C1Fe2	#58	ICSD_76826	binary_carbide_ICSD_frequ
1219.AB/BA	hP4	P6_{3}/mmc		C10s1	#194	ICSD_168278	binary_carbide_ICSD_frequ
1220.AB/BA	oP12	Pbcn		C1V2	#60	ICSD_9965	binary_carbide_ICSD_frequ
1221.AB/BA	mS28	C2/c		C2Fe5	#15	ICSD_43194	binary_carbide_ICSD_frequ
1222.AB/BA	hP3	P-6m2		C20s1	#187	ICSD_168279	binary_carbide_ICSD_frequ
1223.AB/BA	hP6	P6_{3}/mmc		C20s1	#194	ICSD_168280	binary_carbide_ICSD_frequ
1224.AB/BA	oP16	Pnma		C2Rb2	#62	ICSD_51529	binary_carbide_ICSD_frequ
1225.AB/BA	cI132	Im-3		C60Sr6	#204	ICSD_75356	binary_carbide_ICSD_frequ
1226.AB/BA	hR7	R3m		A14C3	#160	ICSD_14397	binary_carbide_ICSD_frequ
1227.AB/BA	cP7	P-43m		As4C3	#215	ICSD_163831	binary_carbide_ICSD_frequ
1228.AB/BA	hR15	R-3m		B13C2	#166	ICSD_446	binary_carbide_ICSD_frequ
1229.AB/BA	tI24	I-4m2		B1C5	#119	ICSD_166553	binary_carbide_ICSD_frequ
1230.AB/BA	oI12	Imm2		B1C5	#44	ICSD_166554	binary_carbide_ICSD_frequ

1231.AB/BA	hP6	P3m1	B1C5	#156	ICSD_166555	binary_carbide_ICSD_freq
1232.AB/BA	aP12	P-1	B1C5	#2	ICSD_166556	binary_carbide_ICSD_freq
1233.AB/BA	tP8	P-4m2	B1C7	#115	ICSD_181952	binary_carbide_ICSD_freq
1234.AB/BA	hP8	P3m1	B1C7	#156	ICSD_181953	binary_carbide_ICSD_freq
1235.AB/BA	cP8	P-43m	B1C7	#215	ICSD_181954	binary_carbide_ICSD_freq
1236.AB/BA	oP8	Pmm2	B1C7	#25	ICSD_181955	binary_carbide_ICSD_freq
1237.AB/BA	hR8	R3m	B1C7	#160	ICSD_181956	binary_carbide_ICSD_freq
1238.AB/BA	hR15	R-3m	B4C1	#166	ICSD_29093	binary_carbide_ICSD_freq
1239.AB/BA	oP24	Pnma	Ba1C2	#62	ICSD_168408	binary_carbide_ICSD_freq
1240.AB/BA	hR3	R-3m	Ba1C2	#166	ICSD_186576	binary_carbide_ICSD_freq
1241.AB/BA	cP126	Pm-3n	Ba3C60	#223	ICSD_70063	binary_carbide_ICSD_freq
1242.AB/BA	cI132	Im-3	C10Cs1	#204	ICSD_657337	binary_carbide_ICSD_freq
1243.AB/BA	tP68	P-42_{1}c	C19Sc15	#114	ICSD_42631	binary_carbide_ICSD_freq
1244.AB/BA	oP16	Pnma	C1Cr3	#62	ICSD_603557	binary_carbide_ICSD_freq
1245.AB/BA	hP3	P6/mmm	C1Fe2	#191	ICSD_162103	binary_carbide_ICSD_freq
1246.AB/BA	oP12	Pnma	C1Fe2	#62	ICSD_187138	binary_carbide_ICSD_freq
1247.AB/BA	tI32	I-4	C1Fe3	#82	ICSD_187142	binary_carbide_ICSD_freq
1248.AB/BA	hP8	P6_{3}22	C1Fe3	#182	ICSD_42542	binary_carbide_ICSD_freq
1249.AB/BA	oP16	Pnma	C1Fe3	#62	ICSD_43522	binary_carbide_ICSD_freq
1250.AB/BA	mP10	P2_{1}/m	C1Fe4	#11	ICSD_187143	binary_carbide_ICSD_freq
1251.AB/BA	tI10	I4/m	C1Fe4	#87	ICSD_187144	binary_carbide_ICSD_freq
1252.AB/BA	cP5	P-43m	C1Fe4	#215	ICSD_44729	binary_carbide_ICSD_freq
1253.AB/BA	oP16	Pnma	C1Mn3	#62	ICSD_603556	binary_carbide_ICSD_freq
1254.AB/BA	cF112	Fd-3m	C1Mn6	#227	ICSD_187037	binary_carbide_ICSD_freq
1255.AB/BA	hP12	P6_{3}/mmc	C1Mo1	#194	ICSD_44987	binary_carbide_ICSD_freq
1256.AB/BA	hP8	P6_{3}/mmc	C1Mo1	#194	ICSD_618298	binary_carbide_ICSD_freq
1257.AB/BA	hP3	P-6m2	C1Mo2	#187	ICSD_43669	binary_carbide_ICSD_freq
1258.AB	hP4	P6_{3}mc	C1Nb1	#186	ICSD_189092	binary_carbide_ICSD_freq
1259.AB/BA	hP4	P6_{3}/mmc	C1Nb1	#194	ICSD_189093	binary_carbide_ICSD_freq
1260.AB/BA	oP12	Pnma	C1Nb2	#62	ICSD_31973	binary_carbide_ICSD_freq
1261.AB/BA	oP12	Pmma	C1Nb2	#51	ICSD_653912	binary_carbide_ICSD_freq
1262.AB/BA	hR8	R-3c	C1Ni3	#167	ICSD_17005	binary_carbide_ICSD_freq
1263.AB/BA	cP8	P2_{1}3	C10s1	#198	ICSD_168277	binary_carbide_ICSD_freq
1264.AB/BA	hP8	P6_{3}/mmc	C1Re1	#194	ICSD_618702	binary_carbide_ICSD_freq
1265.AB/BA	hP6	P6_{3}/mmc	C1Re2	#194	ICSD_180376	binary_carbide_ICSD_freq
1266.AB/BA	hR4	R-3m	C1Ru1	#166	ICSD_188285	binary_carbide_ICSD_freq
1267.AB/BA	hP3	P-3m1	C1Sc2	#164	ICSD_280743	binary_carbide_ICSD_freq
1268.AB	hP10	P3m1	C1Si1	#156	ICSD_107204	binary_carbide_ICSD_frequenc
1269.AB	hP12	P6_{3}mc	C1Si1	#186	ICSD_15325	binary_carbide_ICSD_frequen
1270.AB	hR16	R3m	C1Si1	#160	ICSD_18136	binary_carbide_ICSD_freq
1271.AB	hR10	R3m	C1Si1	#160	ICSD_24168	binary_carbide_ICSD_freq
1272.AB	hP8	P6_{3}mc	C1Si1	#186	ICSD_24170	binary_carbide_ICSD_freq
1273.AB	hP4	P6_{3}mc	C1Si1	#186	ICSD_24261	binary_carbide_ICSD_freq
1274.AB	hP16	P6_{3}mc	C1Si1	#186	ICSD_24630	binary_carbide_ICSD_freq
1275.AB	hR18	R3m	C1Si1	#160	ICSD_24631	binary_carbide_ICSD_freq
1276.AB	hP38	P3m1	C1Si1	#156	ICSD_27635	binary_carbide_ICSD_freq
1277.AB	hP28	P3m1	C1Si1	#156	ICSD_28303	binary_carbide_ICSD_freq
1278.AB	hP20	P3m1	C1Si1	#156	ICSD_38150	binary_carbide_ICSD_freq
1279.AB	hR14	R3m	C1Si1	#160	ICSD_42513	binary_carbide_ICSD_freq
1280.AB	hP32	P6_{3}mc	C1Si1	#186	ICSD_42858	binary_carbide_ICSD_freq
1281.AB	hP36	P3m1	C1Si1	#156	ICSD_42859	binary_carbide_ICSD_freq
1282.AB	hP42	P3m1	C1Si1	#156	ICSD_43827	binary_carbide_ICSD_freq
1283.AB/BA	cF48	Fd-3m	C1Ti2	#227	ICSD_77473	binary_carbide_ICSD_freq
1284.AB/BA	hP9	P-31m	C1W2	#162	ICSD_162419	binary_carbide_ICSD_freq
1285.AB/BA	oP12	Pbcn	C1W2	#60	ICSD_43017	binary_carbide_ICSD_freq
1286.AB/BA	mP12	P2_{1}/c	C2Ca1	#14	ICSD_24074	binary_carbide_ICSD_freq
1287.AB/BA	cP12	Pn-3m	C2Ca1	#224	ICSD_31092	binary_carbide_ICSD_freq
1288.AB/BA	mS12	C2/m	C2Ca1	#12	ICSD_54185	binary_carbide_ICSD_freq
1289.AB/BA	aP12	P-1	C2Ca1	#2	ICSD_66663	binary_carbide_ICSD_freq
1290.AB/BA	oP20	Pnma	C2Cr3	#62	ICSD_15086	binary_carbide_ICSD_freq
1291.AB/BA	oS20	Cmcm	C2Cr3	#63	ICSD_57009	binary_carbide_ICSD_freq
1292.AB/BA	oP20	Pnma	C2Cr3	#62	ICSD_653958	binary_carbide_ICSD_freq
1293.AB/BA	oP16	Pnma	C2Cs2	#62	ICSD_51531	binary_carbide_ICSD_freq
1294.AB/BA	hP12	P-62m	C2Cs2	#189	ICSD_51533	binary_carbide_ICSD_freq
1295.AB/BA	mS12	C2/c	C2Eu1	#15	ICSD_380495	binary_carbide_ICSD_freq

1296.AB/BA	mS28	C2/c	C2Fe5	#15	ICSD_423888	binary_carbide_ICSD_freq
1297.AB/BA	mS28	C2/c	C2Fe5	#15	ICSD_89328	binary_carbide_ICSD_freq
1298.AB/BA	mS12	C2/m	C2Ir1	#12	ICSD_181488	binary_carbide_ICSD_freq
1299.AB/BA	tI12	I4/mcm	C2Ir1	#140	ICSD_181489	binary_carbide_ICSD_freq
1300.AB/BA	tI6	I4/mmm	C2Ir1	#139	ICSD_181490	binary_carbide_ICSD_freq
1301.AB/BA	tI32	I4_{1}/acd	C2K2	#142	ICSD_36142	binary_carbide_ICSD_freq
1302.AB/BA	tI64	I4_{1}/acd	C2K2	#142	ICSD_89528	binary_carbide_ICSD_freq
1303.AB/BA	oI8	Immm	C2Li2	#71	ICSD_25705	binary_carbide_ICSD_freq
1304.AB/BA	tP6	P4_{2}/mmm	C2Mg1	#136	ICSD_88057	binary_carbide_ICSD_freq
1305.AB/BA	mS28	C2/c	C2Mn5	#15	ICSD_618246	binary_carbide_ICSD_freq
1306.AB/BA	mS28	C2/c	C2Mn5	#15	ICSD_69535	binary_carbide_ICSD_freq
1307.AB/BA	cP12	P4_{3}32	C2Na1	#212	ICSD_186177	binary_carbide_ICSD_freq
1308.AB/BA	tI32	I4_{1}/acd	C2Na2	#142	ICSD_28066	binary_carbide_ICSD_freq
1309.AB/BA	oI8	Immm	C2Na2	#71	ICSD_95835	binary_carbide_ICSD_freq
1310.AB/BA	hP6	P6_{3}/mmc	C2Re1	#194	ICSD_184660	binary_carbide_ICSD_freq
1311.AB/BA	tI6	I4/mmm	C2Re1	#139	ICSD_184661	binary_carbide_ICSD_freq
1312.AB/BA	tP3	P4/mmm	C2Re1	#123	ICSD_184664	binary_carbide_ICSD_freq
1313.AB/BA	tP6	P4_{2}/mmc	C2Si1	#131	ICSD_187721	binary_carbide_ICSD_freq
1314.AB/BA	mS12	C2/c	C2Th1	#15	ICSD_26568	binary_carbide_ICSD_freq
1315.AB/BA	tP6	P4_{2}/mmc	C2Th1	#131	ICSD_77469	binary_carbide_ICSD_freq
1316.AB/BA	hP20	P6_{3}mc	C3Fe7	#186	ICSD_76830	binary_carbide_ICSD_freq
1317.AB/BA	oP16	Pnma	C3Ir1	#62	ICSD_181492	binary_carbide_ICSD_freq
1318.AB/BA	oP16	Pbam	C3Ir5	#55	ICSD_181485	binary_carbide_ICSD_freq
1319.AB/BA	oP10	Pnmm	C3Mg2	#58	ICSD_71941	binary_carbide_ICSD_freq
1320.AB/BA	cP7	Pm-3m	C3Nb4	#221	ICSD_42758	binary_carbide_ICSD_freq
1321.AB/BA	tP20	P-4c2	C3Os2	#116	ICSD_168275	binary_carbide_ICSD_freq
1322.AB/BA	oP40	Pbcn	C3Os2	#60	ICSD_168276	binary_carbide_ICSD_freq
1323.AB/BA	cI28	I-43d	C3Sc4	#220	ICSD_42760	binary_carbide_ICSD_freq
1324.AB/BA	mP10	P2_{1}/c	C4Ir1	#14	ICSD_181493	binary_carbide_ICSD_freq
1325.AB/BA	oF20	Ccce	C4Ir1	#68	ICSD_181496	binary_carbide_ICSD_freq
1326.AB/BA	tP5	P4/nbm	C4Ir1	#125	ICSD_181497	binary_carbide_ICSD_freq
1327.AB/BA	oS40	P6_{3}/mmc	C4Ir1	#194	ICSD_181498	binary_carbide_ICSD_freq
1328.AB/BA	tP36	P-4c2	C5Ir4	#116	ICSD_181486	binary_carbide_ICSD_freq
1329.AB/BA	mS22	C2/m	C5Nb6	#12	ICSD_20695	binary_carbide_ICSD_freq
1330.AB/BA	hR13	R-3m	C5Ti8	#166	ICSD_20822	binary_carbide_ICSD_freq
1331.AB/BA	hP33	P3_{1}12	C5V6	#151	ICSD_71098	binary_carbide_ICSD_freq
1332.AB/BA	cP126	Pm-3	C6OSr3	#200	ICSD_75354	binary_carbide_ICSD_freq
1333.AB/BA	hP14	P6_{3}/mmc	C6Eu1	#194	ICSD_169041	binary_carbide_ICSD_freq
1334.AB/BA	hP14	P6_{3}/mmc	C6Yb1	#194	ICSD_601565	binary_carbide_ICSD_freq
1335.AB/BA	mP44	P2_{1}/c	C7Ho4	#14	ICSD_74817	binary_carbide_ICSD_freq
1336.AB/BA	cI40	Im-3m	C7Ir3	#229	ICSD_181491	binary_carbide_ICSD_freq
1337.AB/BA	cP60	P4_{3}32	C7V8	#212	ICSD_22177	binary_carbide_ICSD_freq
1338.AB/BA	cP60	P4_{3}32	C7V8	#212	ICSD_43259	binary_carbide_ICSD_freq
1339.AB/BA	hP9	P6/mmm	C8Cs1	#191	ICSD_74641	binary_carbide_ICSD_freq
1340.AB/BA	oF72	Fddd	C8K1	#70	ICSD_70020	binary_carbide_ICSD_freq
1341.AB/BA	oF72	Fddd	C8Rb1	#70	ICSD_200563	binary_carbide_ICSD_freq

*** TERNARIES

T0001.A2BC/AB2C/ABC2		cF16	Fm(-3)m	AlCu2Mn-Heusler	#225	Navy [Wyckoff A^C, 3 prot
T0001[-tet[+,-]*%].A2BC/AB2C/ABC2		cF16	Fm(-3)m	AlCu2Mn-Heusler-tet*%	#225	Navy [Wyckoff A^C, 3 prot
T0002.A2BC/AB2C/ABC2		cF16	F-43m	Cu1Li2Sn1-antiHeusler	#216	ICSD_15130 [Wyckoff A^C, .
T0002[-tet[+,-]*%].A2BC/AB2C/ABC2		cF16	F-43m	Cu1Li2Sn1-antiHeusler-tet*%	#216	ICSD_15130 [Wyckoff A^C, .
T0001.{ABC}		cF16	Fm(-3)m	AlCu2Mn-Heusler	#225	Navy [Wyckoff A^C, 3 prot
T0001[-tet[+,-]*%].{ABC}		cF16	Fm(-3)m	AlCu2Mn-Heusler-tet*%	#225	Navy [Wyckoff A^C, 3 prot
T0002.{ABC}		cF16	F-43m	Cu1Li2Sn1-antiHeusler	#216	ICSD_15130 [Wyckoff A^C, .
T0002[-tet[+,-]*%].{ABC}		cF16	F-43m	Cu1Li2Sn1-antiHeusler-tet*%	#216	ICSD_15130 [Wyckoff A^C, .
T0003.{ABC}		cF12	F-43m	AgAsMg-halfHeusler	C1b #216	ICSD_43819
T0003[-tet[+,-]*%].{ABC}		cF12	F-43m	AgAsMg-halfHeusler-tet*%	C1b #216	ICSD_43819 TET distorted
T0004.{ABC}	oP12	Pnma	Co1Ge1Mn1_ICSD_52968	#62	ICSD_52968	
T0005.{ABC}	hP6	P63/mmc	Co1Ge1Mn1_ICSD_623495	#194	ICSD_623495	
T0006.{ABC}	hP12	P63/mmc	Co3Ge1Mn2_ICSD_52972	#194	ICSD_52972	
T0007.{ABC}	oP12	Pnma	Cl1La1Se1_ICSD_425686	#62	ICSD_425686	
T0008.{ABC}	oP12	Pnma	Cd1Na1P1 Co2Si1_ICSD_44858	#62	ICSD_44858	
T0009.{ABC}	cP5	Pm-3m	perovskite	#221		

T0010.{ABC}	cF24	F-43m	Cu4MgSn	C15b	#216	ICSD_108141
T0011.{ABC}	tI10	I4/mmm	As2Ce1Pd2		#139	ICSD_604354

*** TERNARY SQS

TS001.ABC/BCA/CBA	oS64	Cmma		SQS_L12	#67	SQS_L12
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*** TERNARY FCC

TFCC001.ABC	hP3	P3m1	ternary_fcc_1	#156	3cell
TFCC002.ABC	oI6	Imm2	ternary_fcc_2	#44	3cell
TFCC003.ABC	tI6	I4mm	ternary_fcc_3	#107	3cell
TFCC004.ABC/BCA/CAB	hR4	R3m	ternary_fcc_4	#160	4cell
TFCC005.ABC/BCA/CAB	oP4	Pmm2	ternary_fcc_5	#25	4cell
TFCC006.ABC/BCA/CAB	mS8	Cm	ternary_fcc_6	#8	4cell
TFCC007.ABC/BCA/CAB	tP4	P4mm	ternary_fcc_7	#99	4cell
TFCC008.ABC/BCA/CAB	tI8	I-4m2	ternary_fcc_8	#119	4cell
TFCC009.ABC/BCA/CAB	hR4	R-3m	ternary_fcc_9	#166	4cell
TFCC010.ABC/BCA/CAB	oP4	Pmmm	ternary_fcc_10	#47	4cell
TFCC011.ABC/BCA/CAB	mS8	C2/m	ternary_fcc_11	#12	4cell
TFCC012.ABC/BCA/CAB	tP4	P4/mmm	ternary_fcc_12	#123	4cell
TFCC013.ABC/BCA/CAB	tI8	I4/mmm	ternary_fcc_13	#139	4cell
TFCC014.ABC/BCA/CAB	mP4	P2/m	ternary_fcc_14	#10	4cell
TFCC015.ABC/BCA/CAB	oS8	Cmmm	ternary_fcc_15	#65	4cell
TFCC016.ABC/BCA/CAB	tP4	P4/mmm	ternary_fcc_16	#123	4cell

*** TERNARY BCC

TBCC001.ABC	oF12	Fmm2	ternary_bcc_1	#42	3cell
TBCC002.ABC	hP3	P3m1	ternary_bcc_2	#156	3cell
TBCC003.ABC	tI6	I4mm	ternary_bcc_3	#107	3cell
TBCC004.ABC/BCA/CAB	oS8	Cmm2	ternary_bcc_4	#35	4cell
TBCC005.ABC/BCA/CAB	mP4	Pm	ternary_bcc_5	#6	4cell
TBCC006.ABC/BCA/CAB	tP4	P4mm	ternary_bcc_6	#99	4cell
TBCC007.ABC/BCA/CAB	oI8	Imm2	ternary_bcc_7	#44	4cell
TBCC008.ABC/BCA/CAB	cF16	F-43m	ternary_bcc_8	#216	4cell same as T0002 (anti-Heusler)
TBCC009.ABC/BCA/CAB	oS8	Cmmm	ternary_bcc_9	#65	4cell
TBCC010.ABC/BCA/CAB	mP4	P2/m	ternary_bcc_10	#10	4cell
TBCC011.ABC/BCA/CAB	tP4	P4/mmm	ternary_bcc_11	#123	4cell
TBCC012.ABC/BCA/CAB	oI8	Cmmm	ternary_bcc_12	#65	4cell
TBCC013.ABC/BCA/CAB	cF16	Fm-3m	ternary_bcc_13	#225	4cell same as T0001 (Heusler)
TBCC014.ABC/BCA/CAB	mS8	C2/m	ternary_bcc_14	#12	4cell
TBCC015.ABC/BCA/CAB	oP4	Pmmm	ternary_bcc_15	#47	4cell
TBCC016.ABC/BCA/CAB	tP4	P4/mmm	ternary_bcc_16	#123	4cell

*** QUATERNARY

Q0001.{ABCD}	cF40	Fm(-3)m	Al1F6K2Na1_ICSD_6027	#225	ICSD_6027 Elpasolite [Wyckoff all dist
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*           aflow - STEFANO CURTAROLO Duke University 2003-2017
*           High-Throughput ab-initio Computing Project
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