SHG in magnetic materials

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There are more than 1795 magnetic phases recorded in MAGNDATA(http://webbdcrista1.ehu.es/magndata/) (we called them are magnetic phases because one magnetic material may have several magnetic structures). Apart from the incommensurate magnetic structures, there are 1655 magnetic phases with BCS-ID 0.1-0.835, 1.0.1-1.0.52, 1.1-1.663, 2.1-2.86, and 3.1-3.19. Then removing duplicate data, there remains 1432 magnetic phases. We find 496 magnetic phases have SHG effect, 451 magnetic phases have the LMO effect, and 100 magnetic phases have both LMO and SHG effects.

I. CLARIFICATION OF SHG IN MAGNDATA DATABASE

TABLE S1: Clarification of SHG in MAGNDATA database (BCS-ID 0.1-0.835, 1.0.1-1.0.52, 1.1-1.663, 2.1-2.86, and 3.1-3.19). The underline wave symbols mean the materials have been appears In front of this table.

BCS-ID	Formula	Parent SG	MSG	MPG	SHG	LMO
0.1	$LaMnO_3$	$Pnma$ (62)	$Pn'ma'$ (62.448)	$m'm'm$	×	✓
0.2	$Cd_2Os_2O_7$	$Fd\bar{3}m$ (227)	$Fd\bar{3}m'$ (227.131)	$m\bar{3}m'$	×	×
0.3	Ca_3LiOsO_6	$R\bar{3}c$ (167)	$C2'/c'$ (15.89)	$2'/m'$	×	✓
0.4	$NiCr_2O_4$	$I4_1/amd$ (141)	$Fd'd'd$ (70.530)	$m'm'm$	×	✓
0.5	Cr_2S_3	$R\bar{3}$ (148)	$P\bar{1}$ (2.4)	$\bar{1}$	×	✓
0.6	$YMnO_3$	$P6_3cm$ (185)	$P6_3cm$ (185.197)	$6mm$	O-woP	×
0.7	$ScMnO_3$	$P6_3cm$ (185)	$P6_3c'm'$ (185.201)	$6m'm'$	BW-woP	✓
0.8	$ScMnO_3$	$P6_3cm$ (185)	$P6_3$ (173.129)	6	O-woP	✓
0.9	GdB_4	$P4/mbm$ (127)	$P4/m'b'm'$ (127.395)	$4/m'm'm'$	PT-wP	×
0.10	$DyFeO_3$	$Pnma$ (62)	$P2_12_12_1$ (19.25)	222	O-wP	×
0.11	$DyFeO_3$	$Pnma$ (62)	$Pn'a'2_1$ (33.148)	$m'm'2$	BW-wP	✓
0.12	$U_3Ru_4Al_{12}$	$P6_3/mmc$ (194)	$Cmcm'$ (63.461)	$m'mm$	PT-wP	×
0.13	$Ca_3Co_{2-x}Mn_xO_6$	$R\bar{3}c$ (167)	$R3c$ (161.69)	$3m$	O-wP	×
0.14	Gd_5Ge_4	$Pnma$ (62)	$Pnm'a$ (62.444)	$m'mm$	PT-wP	×
0.15	MnF_2	$P4_2/mnm$ (136)	$P4_2'/mnm'$ (136.499)	$4'/mm'm$	×	×
0.16	$EuTiO_3$	$I4/mcm$ (140)	$Fm'mm$ (69.523)	$m'mm$	PT-wP	×
0.17	$FePO_4$	$Pnma$ (62)	$P2_12_12_1$ (19.25)	222	O-wP	×
0.18	$BaMn_2As_2$	$I4/mmm$ (139)	$I4'/m'm'm$ (139.536)	$4'/m'm'm$	PT-wP	×
0.19	$MnTiO_3$	$R\bar{3}$ (148)	$R\bar{3}'$ (148.19)	$\bar{3}'$	PT-wP	×
0.20	$MnTe_2$	$Pa\bar{3}$ (205)	$Pa\bar{3}$ (205.33)	$m\bar{3}$	×	×
0.21	$PbNiO_3$	$R3c$ (161)	$R3c$ (161.69)	$3m$	O-woP	×
0.22	DyB_4	$P4/mbm$ (127)	$Pb'am$ (55.355)	$m'mm$	PT-wP	×
0.23	$Ca_3Mn_2O_7$	$Cmc2_1$ (36)	$Cm'c2_1'$ (36.174)	$m'm2'$	BW-woP	✓
0.24	$LiMnPO_4$	$Pnma$ (62)	$Pn'm'a'$ (62.449)	$m'm'm'$	PT-wP	×
0.25	$NaOsO_3$	$Pnma$ (62)	$Pn'ma'$ (62.448)	$m'm'm$	×	✓
0.26	$TmAgGe$	$P\bar{6}2m$ (189)	$Am'm'2$ (38.191)	$m'm'2$	BW-woP	✓
0.27	YFe_4Ge_2	$Pnnm$ (58)	$Pn'n'm'$ (58.399)	$m'm'm'$	PT-wP	×
0.28	$LiFeSi_2O_6$	$P2_1/c$ (14)	$P2_1/c'$ (14.78)	$2/m'$	PT-wP	×
0.29	$Er_2Ti_2O_7$	$Fd\bar{3}m$ (227)	$I4_1'/am'd$ (141.554)	$4'/mm'm$	×	×
0.30	$YbMnO_3$	$P6_3cm$ (185)	$P6_3'c'm$ (185.199)	$6'mm'$	BW-woP	×
0.31	$HoMnO_3$	$P6_3cm$ (185)	$P6_3c'm'$ (185.201)	$6m'm'$	BW-woP	✓
0.32	$HoMnO_3$	$P6_3cm$ (185)	$P6_3cm$ (185.197)	$6mm$	O-woP	×
0.33	$HoMnO_3$	$P6_3cm$ (185)	$P6_3cm$ (185.197)	$6mm$	O-woP	×
0.34	$La_{0.5}Sr_{0.5}FeO_{2.5}F_{0.5}$	$Pnma$ (062)	$Pn'ma'$ (62.448)	$m'm'm$	×	✓
0.35	Cu_2OSeO_3	$P2_13$ (198)	$R3$ (146.10)	3	O-woP	✓
0.36	NiF_2	$P4_2/mnm$ (136)	$Pnn'm'$ (58.398)	$m'm'm$	×	✓
0.37	$U_3Al_2Si_3$	$I4$ (79)	$C2'$ (5.15)	$2'$	BW-woP	✓

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TABLE S1 – continued from previous page

BCS-ID	Formula	Parent	MSG	MPG	SHG type	LMO
0.38	$GaFeO_3$	$Pna2_1$ (33)	$Pna'2'_1$ (33.147)	$m'm2'$	BW-woP	✓
0.39	Nd_2NaRuO_6	$P2_1/n$ (14)	$P2_1/c$ (14.75)	$2/m$	×	✓
0.40	Mn_2O_3-alpha	$Pbca$ (61)	$Pbca$ (61.433)	mmm	×	×
0.41	Mn_2O_3-alpha	$Pbca$ (61)	$Pbca$ (61.433)	mmm	×	×
0.42	$HoMnO_3$	$P6_3cm$ (185)	$P6'_3c'm$ (185.199)	$6'mm'$	BW-woP	×
0.43	$HoMnO_3$	$P6_3cm$ (185)	$P6'_3cm'$ (185.2)	$6'mm'$	BW-woP	×
0.44	$YMnO_3$	$P6_3cm$ (185)	$P6'_3$ (173.131)	$6'$	BW-woP	×
0.45	La_2NiO_4	$P4_2/ncm$ (138)	$Pc'c'n$ (56.369)	$m'm'm$	×	✓
0.46	$CaBaCo_4O_7$	$Pbn2_1$ (33)	$Pna'2'_1$ (33.147)	$m'm2'$	BW-woP	✓
0.47	$Gd_2Sn_2O_7$	$Fd\bar{3}m$ (227)	$I4'_1/amd'$ (141.555)	$4'/mm'm$	×	×
0.48	$Tb_2Sn_2O_7$	$Fd\bar{3}m$ (227)	$I4_1/am'd'$ (141.557)	$4/mm'm'$	×	✓
0.49	$Ho_2Ru_2O_7$	$Fd\bar{3}m$ (227)	$I4_1/am'd'$ (141.557)	$4/mm'm'$	×	✓
0.50	$MnTiO_3$	$R3c$ (161)	Cc' (9.39)	m'	BW-woP	✓
0.51	$Ho_2Ru_2O_7$	$Fd\bar{3}m$ (227)	$I4_1/am'd'$ (141.557)	$4/mm'm'$	×	✓
0.52	$K_yFe_{2-x}Se_2$	$I4/m$ (87)	$C2'/m'$ (12.62)	$2'/m'$	×	✓
0.53	$Rb_yFe_{2-x}Se_2$	$I4/m$ (87)	$C2'/m'$ (12.62)	$2'/m'$	×	✓
0.54	$Rb_yFe_{2-x}Se_2$	$I4/m$ (87)	$I4/m'$ (87.78)	$4/m'$	PT-wP	×
0.55	K_yFe_2-xSe_2	$I4/m$ (87)	$I4/m'$ (87.78)	$4/m'$	PT-wP	×
0.56	$Ba_2CoGe_2O_7$	$P\bar{4}2_1m$ (113)	$Cm'm2'$ (35.167)	$m'm2'$	BW-woP	✓
0.57	$ScFeO_3$	$R3c$ (161)	Cc' (9.39)	m'	BW-woP	✓
0.58	$CoAl_2O_4$	$Fd\bar{3}m$ (227)	$I4'_1/a'm'd$ (141.556)	$4'/m'm'm$	PT-wP	×
0.59	Cr_2O_3	$R\bar{3}c$ (167)	$R\bar{3}'c'$ (167.106)	$\bar{3}'m'$	PT-wP	×
0.60	$[NH_2(CH_3)_2]_n[Fe^{III}Fe^{II}(HCOO)_6]_n$	$R\bar{3}c$ (167)	$R\bar{3}c'$ (167.107)	$\bar{3}m'$	×	✓
0.61	$Li_2FeP_2O_7$	$P2_1/c$ (14)	$P2_1/c$ (14.75)	$2/m$	×	✓
0.62	$SrMn_2V_2O_8$	$I4_1cd$ (110)	$Ib'a2'$ (45.237)	$m'm2'$	BW-woP	✓
0.63	Ho_2CrSbO_7	$Fd\bar{3}m$ (227)	$I4_1/am'd'$ (141.557)	$4/mm'm'$	×	✓
0.64	MnV_2O_4	$I4_1/a$ (88)	$I4_1/a$ (88.81)	$4/m$	×	✓
0.65	Fe_2O_3-alpha	$R\bar{3}c$ (167)	$C2'/c'$ (15.89)	$2'/m'$	×	✓
0.66	Fe_2O_3-alpha	$R\bar{3}c$ (167)	$P\bar{1}$ (2.4)	$\bar{1}$	×	✓
0.67	$BiFe_{0.5}Sc_{0.5}O_3$	$Ima2$ (46)	$Im'a2'$ (46.243)	$m'm2'$	BW-woP	✓
0.68	$BiFe_{0.5}Sc_{0.5}O_3$	$Pnma$ (62)	$Pn'm'a$ (62.446)	$m'm'm$	×	✓
0.69	$Co_4(OH)_2(C_{10}H_{16}O_2)_3$	$P2_1/c$ (14)	$P2'_1/c'$ (14.79)	$2'/m'$	×	✓
0.70	$Na_3Co(CO_3)_2Cl$	$Fd\bar{3}$ (203)	$Fd\bar{3}$ (203.26)	$m\bar{3}$	×	×
0.71	$Li_2Ni(SO_4)_2$	$Pbca$ (61)	$Pb'c'a'$ (61.437)	$m'm'm'$	PT-wP	×
0.72	$CaMnBi_2$	$P4/nmm$ (129)	$P4'/n'm'm$ (129.416)	$4'/m'm'm$	PT-wP	×
0.73	$SrMnBi_2$	$I4/mmm$ (139)	$I4'/m'm'm$ (139.536)	$4'/m'm'm$	PT-wP	×
0.74	$Mn_3Cu_{0.5}Ge_{0.5}N$	$Pm\bar{3}m$ (221)	$R\bar{3}m$ (166.97)	$\bar{3}m$	×	×
0.75	Cr_2WO_6	$P4_2/mnm$ (136)	$Pn'nm$ (58.395)	$m'mm$	PT-wP	×
0.76	Cr_2TeO_6	$P4_2/mnm$ (136)	$Pn'nm$ (58.395)	$m'mm$	PT-wP	×
0.77	$Tb_2Ti_2O_7$	$Fd\bar{3}m$ (227)	$R\bar{3}m'$ (166.101)	$\bar{3}m'$	×	✓
0.78	NiN_2O_6	$R\bar{3}$ (148)	$R\bar{3}$ (148.17)	$\bar{3}$	×	✓
0.79	$CaIrO_3$	$Cmcm$ (63)	$Cm'cm'$ (63.464)	$m'm'm$	×	✓
0.80	U_2Pd_2In	$P4/mbm$ (127)	$P4'/m'bm'$ (127.394)	$4'/m'm'm$	PT-wP	×
0.81	U_2Pd_2Sn	$P4/mbm$ (127)	$P4'/m'bm'$ (127.394)	$4'/m'm'm$	PT-wP	×
0.82	Gd_2CuO_4	$Aeam$ (64)	$Cm'ca'$ (64.476)	$m'm'm$	×	✓
0.83	$LiFeP_2O_7$	$P2_1$ (4)	$P2_1$ (4.7)	2	O-woP	✓
0.84	Mn_2FeMoO_6	$R3$ (146)	$R3$ (146.10)	3	O-woP	✓
0.85	$KCo_4(PO_4)_3$	$Pnnm$ (58)	$Pnn'm'$ (58.398)	$m'm'm$	×	✓
0.86	$KMn_4(PO_4)_3$	$Pnam$ (62)	$Pnma'$ (62.445)	$m'mm$	PT-wP	×
0.87	$NaFePO_4$	$Pnma$ (62)	$Pnma'$ (62.445)	$m'mm$	PT-wP	×
0.88	$LiNiPO_4$	$Pnma$ (62)	$Pnm'a$ (62.444)	$m'mm$	PT-wP	×
0.89	$BaMn_2Bi_2$	$I4/mmm$ (139)	$I4'/m'm'm$ (139.536)	$4'/m'm'm$	PT-wP	×
0.90	$Rb_2Fe_2O(AsO_4)_2$	$Pnma$ (62)	$Pnma$ (62.441)	mmm	×	×
0.91	$Rb_2Fe_2O(AsO_4)_2$	$Pnma$ (62)	$Pn'ma'$ (62.448)	$m'm'm$	×	✓
0.92	$CaMn_2Sb_2$	$P\bar{3}m1$ (164)	$C2'/m$ (12.60)	$2'/m$	PT-wP	×

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TABLE S1 – continued from previous page

BCS-ID	Formula	Parent	MSG	MPG	SHG type	LMO
0.93	$Ca_2Fe_2O_5$	$Pcmn$ (62)	$Pcm'n'$ (62.446)	$m'm'm$	×	✓
0.94	$TeNiO_3$	$Pnma$ (62)	$Pn'm'a$ (62.446)	$m'm'm$	×	✓
0.95	$LiFePO_4$	$Pnma$ (62)	$Pnma'$ (62.445)	$m'mm$	PT-wP	×
0.96	$CoSO_4$	$Pnma$ (62)	$Pnma$ (62.441)	mmm	×	×
0.97	$FeSb_2O_4$	$P4_2/mbc$ (135)	$Pmc2_1$ (26.66)	$mm2$	O-wP	×
0.98	$YBaMn_2O_{5.5}$	$Icam$ (72)	$Ib'a'm$ (72.543)	$m'm'm$	×	✓
0.99	$YBaMn_2O_{5.5}$	$Icam$ (72)	$C2/m$ (12.58)	$2/m$	×	✓
0.100	$YCr_{0.5}Mn_{0.5}O_3$	$Pnma$ (62)	$Pn'ma'$ (62.448)	$m'm'm$	×	✓
0.101	Mn_2GeO_4	$Pnma$ (62)	$Pn'm'a$ (62.446)	$m'm'm$	×	✓
0.102	Mn_2GeO_4	$Pnma$ (62)	$Pnma$ (62.441)	mmm	×	×
0.103	Mn_2GeO_4	$Pnma$ (62)	$P2_1/c$ (14.75)	$2/m$	×	✓
0.104	$ErVO_3$	$Pbnm$ (62)	$P2_1'/m'$ (11.54)	$2'/m'$	×	✓
0.105	$ErVO_3$	$Pbnm$ (62)	$P2_1/c$ (14.75)	$2/m$	×	✓
0.106	$DyVO_3$	$Pbnm$ (62)	$P2_1'/m'$ (11.54)	$2'/m'$	×	✓
0.107	$Ho_2Ge_2O_7$	$P4_12_12$ (92)	$P4_12_12$ (92.111)	422	O-woP	×
0.108	Mn_3Ir	$Pm\bar{3}m$ (221)	$R\bar{3}m'$ (166.101)	$\bar{3}m'$	×	✓
0.109	Mn_3Pt	$Pm\bar{3}m$ (221)	$R\bar{3}m'$ (166.101)	$\bar{3}m'$	×	✓
0.110	Cr_2O_3	$R\bar{3}c$ (167)	$C2'/c$ (15.87)	$2'/m$	PT-wP	×
0.111	$Co_4Nb_2O_9$	$P\bar{3}c1$ (165)	$P\bar{3}'c'1$ (165.94)	$\bar{3}'m'$	PT-wP	×
0.112	$FeBO_3$	$R\bar{3}c$ (167)	$C2'/c'$ (15.89)	$2'/m'$	×	✓
0.113	$NiCO_3$	$R\bar{3}c$ (167)	$C2/c$ (15.85)	$2/m$	×	✓
0.114	$CoCO_3$	$R\bar{3}c$ (167)	$C2/c$ (15.85)	$2/m$	×	✓
0.115	$MnCO_3$	$R\bar{3}c$ (167)	$C2/c$ (15.85)	$2/m$	×	✓
0.116	$FeCO_3$	$R\bar{3}c$ (167)	$R\bar{3}c$ (167.103)	$\bar{3}m$	×	×
0.117	$LuFeO_3$	$P6_3cm$ (185)	$P6_3c'm'$ (185.201)	$6m'm'$	BW-woP	✓
0.118	$Ba_5Co_5ClO_{13}$	$P6_3/mmc$ (194)	$P6_3'/m'm'c$ (194.268)	$6'/m'mm'$	×	×
0.119	$CoSe_2O_5$	$Pbcn$ (60)	$Pb'cn$ (60.419)	$m'mm$	PT-wP	×
0.120	$LiFe(SO_4)_2$	$P2_1/c$ (14)	$P2_1/c$ (14.75)	$2/m$	×	✓
0.121	$Li_2Co(SO_4)_2$	$P2_1/c$ (14)	$P2_1'/c'$ (14.79)	$2'/m'$	×	✓
0.122	$Li_2Mn(SO_4)_2$	$P2_1/c$ (14)	$P2_1/c$ (14.75)	$2/m$	×	✓
0.123	Mn_3NiN	$Pm\bar{3}m$ (221)	$R\bar{3}$ (148.17)	$\bar{3}$	×	✓
0.124	Mn_3NiN	$Pm\bar{3}m$ (221)	$R\bar{3}$ (148.17)	$\bar{3}$	×	✓
0.125	$MnGeO_3$	$R\bar{3}$ (148)	$R\bar{3}'$ (148.19)	$\bar{3}'$	PT-wP	×
0.126	$NpCo_2$	$Fd\bar{3}m$ (227)	$I4_1'/a'm'd$ (141.556)	$4'/m'm'm$	PT-wP	×
0.127	$Dy_3Al_5O_{12}$	$Ia\bar{3}d$ (230)	$Ia\bar{3}d'$ (230.148)	$m\bar{3}m'$	×	×
0.128	$FeSO_4F$	$C2/c$ (15)	$C2'/c'$ (15.89)	$2'/m'$	×	✓
0.129	$Cu_3Mo_2O_9$	$Pnma$ (62)	$P2_1'2_12_1$ (19.27)	$2'2'2$	BW-wP	✓
0.130	$Cu_3Mo_2O_9$	$Pnma$ (62)	$Pm'c2_1'$ (26.68)	$m'm2'$	BW-wP	✓
0.131	$Mn(N(CN_2))_2$	$Pnnm$ (58)	$Pnn'm'$ (58.398)	$m'm'm$	×	✓
0.132	$Fe(N(CN_2))_2$	$Pnnm$ (58)	$Pnn'm'$ (58.398)	$m'm'm$	×	✓
0.133	$Ni_3B_7O_{13}Cl$	$Pca2_1$ (29)	$Pc'a2_1'$ (29.101)	$m'm2'$	BW-woP	✓
0.134	$Mn_3B_7O_{13}I$	$Pca2_1$ (29)	$Pc'a2_1'$ (29.101)	$m'm2'$	BW-woP	✓
0.135	$Ni_3B_7O_{13}Br$	$Pca2_1$ (29)	$Pc'a2_1'$ (29.101)	$m'm2'$	BW-woP	✓
0.136	$Co_3B_7O_{13}Br$	$Pca2_1$ (29)	$Pc'a2_1'$ (29.101)	$m'm2'$	BW-woP	✓
0.137	$Cu_2V_2O_7$	$Fdd2$ (43)	$Fd'd'2$ (43.227)	$m'm'2$	BW-woP	✓
0.138	$BiCrO_3$	$C2/c$ (15)	$C2/c$ (15.85)	$2/m$	×	✓
0.139	$BiCrO_3$	$C2/c$ (15)	$P\bar{1}$ (2.4)	$\bar{1}$	×	✓
0.140	$LuFe_4Ge_2$	$P4_2/mnm$ (136)	$Pn'n'm'$ (58.399)	$m'm'm'$	PT-wP	×
0.141	Tb_5Ge_4	$Pnma$ (62)	$Pnm'a$ (62.444)	$m'mm$	PT-wP	×
0.142	Fe_2TeO_6	$P4_2/mnm$ (136)	$P4_2/m'n'm'$ (136.503)	$4/m'm'm'$	PT-wP	×
0.143	Cr_2TeO_6	$P4_2/mnm$ (136)	$Pn'nm$ (58.395)	$m'mm$	PT-wP	×
0.144	Cr_2WO_6	$P4_2/mnm$ (136)	$Pn'nm$ (58.395)	$m'mm$	PT-wP	×
0.145	Co_3TeO_6	$C2/c$ (15)	$C2'/c$ (15.87)	$2'/m$	PT-wP	×
0.146	$EuZrO_3$	$Pnma$ (62)	$Pnm'a$ (62.444)	$m'mm$	PT-wP	×
0.147	$EuZrO_3$	$Pnma$ (62)	$Pn'm'a'$ (62.449)	$m'm'm'$	PT-wP	×
0.148	La_2LiRuO_6	$P2_1/n$ (14)	$P2_1/c$ (14.75)	$2/m$	×	✓

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TABLE S1 – continued from previous page

BCS-ID	Formula	Parent	MSG	MPG	SHG type	LMO
0.149	$Nd_3Ru_4Al_{12}$	$P6_3/mmc$ (194)	$Cm'c'm$ (63.462)	$m'm'm$	×	✓
0.15	NiS_2	$Pa\bar{3}$ (205)	$Pa\bar{3}$ (205.33)	$m\bar{3}$	×	×
0.151	$Tm_2Mn_2O_7$	$Fd\bar{3}m$ (227)	$I4_1/am'd'$ (141.557)	$4/mm'm'$	×	✓
0.152	$LiFePO_4$	$Pnma$ (62)	$P2_1/c'$ (14.78)	$2/m'$	PT-wP	×
0.153	Bi_2RuMnO_7	$Fd\bar{3}m$ (227)	$Fd'd'd$ (70.530)	$m'm'm$	×	✓
0.154	$Er_2Ru_2O_7$	$Fd\bar{3}m$ (227)	$I4_1'/am'd$ (141.554)	$4'/mm'm$	×	×
0.155	$CaMnGe_2O_6$	$C2/c$ (15)	$P\bar{1}'$ (2.6)	$\bar{1}'$	PT-wP	×
0.156	$CaMnGe_2O_6$	$C2/c$ (15)	$C2'/c$ (15.87)	$2'/m$	PT-wP	×
0.157	$Yb_2Sn_2O_7$	$Fd\bar{3}m$ (227)	$I4_1/am'd'$ (141.557)	$4/mm'm'$	×	✓
0.158	$Yb_2Ti_2O_7$	$Fd\bar{3}m$ (227)	$I4_1/am'd'$ (141.557)	$4/mm'm'$	×	✓
0.159	$DyCoO_3$	$Pbnm$ (62)	$Pn'm'a'$ (62.449)	$m'm'm'$	PT-wP	×
0.160	$TbCoO_3$	$Pbnm$ (62)	$Pnm'a$ (62.444)	$m'mm$	PT-wP	×
0.161	$CoSe_2O_5$	$Pbcn$ (60)	$Pb'cn$ (60.419)	$m'mm$	PT-wP	×
0.162	$NdCrTiO_5$	$Pbam$ (55)	$Pbam'$ (55.356)	$m'mm$	PT-wP	×
0.163	$MnPS_3$	$C2/m$ (12)	$C2'/m$ (12.60)	$2'/m$	PT-wP	×
0.164	Y_2MnCoO_6	$P2_1/c$ (14)	$P2_1'/c'$ (14.79)	$2'/m'$	×	✓
0.165	$SrMn(VO_4)(OH)$	$P2_12_12_1$ (19)	$P2_1$ (4.7)	2	O-woP	✓
0.166	Ce_2PdGe_3	$P4_2/mmc$ (131)	$P4_2'/m'm'c$ (131.440)	$4'/m'm'm$	PT-wP	×
0.167	$Nd_3Sb_3Mg_2O_{14}$	$R\bar{3}m$ (166)	$R\bar{3}m'$ (166.101)	$\bar{3}m'$	×	✓
0.168	$NH_4Fe_2F_6$	$Pnma$ (62)	$Pnma$ (62.441)	mmm	×	×
0.169	U_3As_4	$I\bar{4}3d$ (220)	$R3c'$ (161.71)	$3m'$	BW-woP	✓
0.170	U_3P_4	$I\bar{4}3d$ (220)	$R3c'$ (161.71)	$3m'$	BW-woP	✓
0.171	$DyScO_3$	$Pnma$ (62)	$Pn'm'a'$ (62.449)	$m'm'm'$	PT-wP	×
0.172	$Y_3Co_{3.25}Al_{0.75}$	$Cmcm$ (63)	$Cm'cm'$ (63.464)	$m'm'm$	×	✓
0.173	$Pr_3Ru_4Al_{12}$	$P6_3/mmc$ (194)	$Cm'c'm$ (63.462)	$m'm'm$	×	✓
0.174	$Pr_3Ru_4Al_{12}$	$P6_3/mmc$ (194)	$C2'/c'$ (15.89)	$2'/m'$	×	✓
0.175	$Ca_2CoSi_2O_7$	$P\bar{4}2_1m$ (113)	$P2_12_1'2'$ (18.19)	$2'2'2$	BW-woP	✓
0.176	$Mn_3Ti_2Te_6$	$P\bar{3}1c$ (163)	$C2'/c'$ (15.89)	$2'/m'$	×	✓
0.177	Mn_3GaN	$Pm\bar{3}m$ (221)	$R\bar{3}m$ (166.97)	$\bar{3}m$	×	×
0.178	CoF_2	$P4_2/mnm$ (136)	$P4_2'/mnm'$ (136.499)	$4'/mm'm$	×	×
0.179	$FeCl_5D_2O(ND_4)_2$	$P2_1/c$ (14)	$P2_1'$ (4.9)	$2'$	BW-wP	✓
0.180	$MnPSe_3$	$R\bar{3}$ (148)	$P\bar{1}'$ (2.6)	$\bar{1}'$	PT-wP	×
0.181	$Nd_{15}Ge_9C_{0.39}$	$P6_3mc$ (186)	$P6_3m'c'$ (186.207)	$6m'm'$	BW-woP	✓
0.182	$KCrF_4$	$Pnma$ (62)	$Pn'ma$ (62.443)	$m'mm$	PT-wP	×
0.183	$KMnFeF_6$	$P4_2bc$ (106)	$Pb'a2'$ (32.137)	$m'm2'$	BW-woP	✓
0.184	Nd_5Si_4	$P4_12_12$ (92)	$P4_12_12'$ (92.114)	$42'2'$	BW-woP	✓
0.185	Nd_5Ge_4	$Pnma$ (62)	$Pnm'a'$ (62.447)	$m'm'm$	×	✓
0.186	$CeMnAsO$	$P4/nmm$ (129)	$P4'/n'm'm$ (129.416)	$4'/m'm'm$	PT-wP	×
0.187	$CeMnAsO$	$P4/nmm$ (129)	$Pm'mn$ (59.407)	$m'mm$	PT-wP	×
0.188	$CeMnAsO$	$P4/nmm$ (129)	$P2'/c$ (13.67)	$2'/m$	PT-wP	×
0.189	$CeMn_2Ge_4O_{12}$	$P4/nbm$ (125)	$P4'/nbm'$ (125.367)	$4'/mm'm$	×	×
0.190	$CeMnCoGe_4O_{12}$	$P4/nbm$ (125)	$Pb'an'$ (50.282)	$m'm'm$	×	✓
0.191	$BaCuF_4$	$Cmc2_1$ (36)	$Cm'c'2_1$ (36.176)	$m'm'2$	BW-woP	✓
0.192	$RbFe_2F_6$	$Pnma$ (62)	$Pnma$ (62.441)	mmm	×	×
0.193	$LiCoPO_4$	$Pnma$ (62)	$Pnma'$ (62.445)	$m'mm$	PT-wP	×
0.194	UPt_2Si_2	$P4/nmm$ (129)	$P4/n'm'm'$ (129.419)	$4/m'm'm'$	PT-wP	×
0.195	$Sr_2Ir_{0.92}Sn_{0.08}O_4$	$I4_1/acd$ (142)	$Ib'c'a$ (73.551)	$m'm'm$	×	✓
0.196	$Co_4Nb_2O_9$	$P\bar{3}c1$ (165)	$C2/c'$ (15.88)	$2/m'$	PT-wP	×
0.197	$Co_4Nb_2O_9$	$P\bar{3}c1$ (165)	$C2/c'$ (15.88)	$2/m'$	PT-wP	×
0.198	$GdVO_4$	$I4_1/amd$ (141)	$I4_1'/a'm'd$ (141.556)	$4'/m'm'm$	PT-wP	×
0.199	Mn_3Sn	$P6_3/mmc$ (194)	$Cmc'm'$ (63.463)	$m'm'm$	×	✓
0.200	Mn_3Sn	$P6_3/mmc$ (194)	$Cm'cm'$ (63.464)	$m'm'm$	×	✓
0.201	$Ca_2PrCr_2NbO_9$	$Pnma$ (62)	$Pn'm'a$ (62.446)	$m'm'm$	×	✓
0.202	$Ca_2PrCr_2TaO_9$	$Pnma$ (62)	$Pn'm'a$ (62.446)	$m'm'm$	×	✓
0.203	Mn_3Ge	$P6_3/mmc$ (194)	$C2'/m'$ (12.62)	$2'/m'$	×	✓

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TABLE S1 – continued from previous page

BCS-ID	Formula	Parent	MSG	MPG	SHG type	LMO
0.204	Ca_2MnReO_6	$P2_1/c$ (14)	$P2_1/c$ (14.75)	$2/m$	×	✓
0.205	Sr_2MnReO_6	$P2_1/c$ (14)	$P2_1'/c'$ (14.79)	$2'/m'$	×	✓
0.206	$Ca_2Fe_{0.885}Cr_{0.125}GaO_6$	$Pbcm$ (62)	$Pn'm'a$ (62.446)	$m'm'm$	×	✓
0.207	$TlFe_{1.6}Se_2$	$I4/m$ (87)	$I4/m$ (87.75)	$4/m$	×	✓
0.208	$TlFe_{1.6}Se_2$	$I4/m$ (87)	$C2'/m$ (12.60)	$2'/m$	PT-wP	×
0.209	$TlFe_{1.6}Se_2$	$I4/m$ (87)	$I4/m'$ (87.78)	$4/m'$	PT-wP	×
0.210	Sr_2CoOsO_6	$B2/n$ (15)	$C2/c$ (15.85)	$2/m$	×	✓
0.211	Ca_2MnO_4	$I4_1/acd$ (142)	$I4_1'/a'cd'$ (142.568)	$4'/m'm'm$	PT-wP	×
0.212	$Sr_2Mn_3As_2O_2$	$I4/mmm$ (139)	$I4'/m'm'm$ (139.536)	$4'/m'm'm$	PT-wP	×
0.213	$Sr_2Mn_2CuAs_2O_2$	$I4/mmm$ (139)	$I4/mm'm'$ (139.537)	$4/mm'm'$	×	✓
0.214	$FePbBiO_4$	$P4_2/mbc$ (135)	$Pmc2_1$ (26.66)	$mm2$	O-wP	×
0.215	$BaNi_2P_2O_8$	$R\bar{3}$ (148)	$P\bar{1}'$ (2.6)	$\bar{1}'$	PT-wP	×
0.216	$SrEr_2O_4$	$Pnma$ (62)	$Pnma'$ (62.445)	$m'mm$	PT-wP	×
0.217	$LiCrGe_2O_6$	$P2_1/c$ (14)	$P2_1'/c$ (14.77)	$2'/m$	PT-wP	×
0.218	Co_2SiO_4	$Pnma$ (62)	$Pnma$ (62.441)	mmm	×	×
0.219	Co_2SiO_4	$Pnma$ (62)	$Pnma$ (62.441)	mmm	×	×
0.220	Mn_2SiO_4	$Pnma$ (62)	$Pn'm'a$ (62.446)	$m'm'm$	×	✓
0.221	Fe_2SiO_4	$Pnma$ (62)	$Pnma$ (62.441)	mmm	×	×
0.222	$CuMnAs$	$P4/nmm$ (129)	$Pm'mn$ (59.407)	$m'mm$	PT-wP	×
0.223	$Cu_{0.95}MnAs$	$Pnma$ (62)	$Pn'ma$ (62.443)	$m'mm$	PT-wP	×
0.224	$Nd_{0.5}Tb_{0.5}Co_2$	$Fd\bar{3}m$ (227)	$C2'/m'$ (12.62)	$2'/m'$	×	✓
0.225	$Nd_{0.5}Tb_{0.5}Co_2$	$Fd\bar{3}m$ (227)	$C2'/m'$ (12.62)	$2'/m'$	×	✓
0.226	$NdCo_2$	$Fd\bar{3}m$ (227)	$C2'/c'$ (15.89)	$2'/m'$	×	✓
0.227	$NdCo_2$	$Fd\bar{3}m$ (227)	$I4_1/am'd'$ (141.557)	$4/mm'm'$	×	✓
0.228	$TbCo_2$	$Fd\bar{3}m$ (227)	$R\bar{3}m'$ (166.101)	$\bar{3}m'$	×	✓
0.229	$Ba_2MnSi_2O_7$	$P\bar{4}2_1m$ (113)	$P\bar{4}2_1m$ (113.267)	$\bar{4}2m$	O-woP	×
0.230	$K_2CoP_2O_7$	$P4_2/mnm$ (136)	$Pn'nm$ (58.395)	$m'mm$	PT-wP	×
0.231	$TmMn_3O_6$	$Pmmn$ (59)	$Pmm'n'$ (59.410)	$m'm'm$	×	✓
0.232	$TmMn_3O_6$	$Pmmn$ (59)	$Pm'm'n$ (59.409)	$m'm'm$	×	✓
0.233	Mn_2FeSbO_6	$R\bar{3}$ (148)	$P\bar{1}$ (2.4)	$\bar{1}$	×	✓
0.234	$MnLaMnSbO_6$	$P4_2/n$ (86)	$P2'/c'$ (13.69)	$2'/m'$	×	✓
0.235	$MnPrMnSbO_6$	$P4_2/n$ (86)	$P42/n$ (86.67)	$4/m$	×	✓
0.236	$CaFe_4Al_8$	$I4/mmm$ (139)	$I4'/mmm'$ (139.535)	$4'/mm'm$	×	×
0.237	$Er_2Sn_2O_7$	$Fd\bar{3}m$ (227)	$I4_1'/amd'$ (141.555)	$4'/mm'm$	×	×
0.238	$Er_2Pt_2O_7$	$Fd\bar{3}m$ (227)	$I4_1'/amd'$ (141.555)	$4'/mm'm$	×	×
0.239	Ca_3LiRuO_6	$R\bar{3}c$ (167)	$C2'/c'$ (15.89)	$2'/m'$	×	✓
0.240	$Er_2Cu_2O_5$	$Pna2_1$ (33)	$Pna2_1$ (33.144)	$mm2$	O-woP	×
0.241	$Y_2Cu_2O_5$	$Pna2_1$ (33)	$Pna2_1$ (33.144)	$mm2$	O-woP	×
0.242	$Tm_2Cu_2O_5$	$Pna2_1$ (33)	$Pn'a'2_1$ (33.148)	$m'm'2$	BW-woP	✓
0.243	$Li_2Fe(SO_4)_2$	$Pbca$ (61)	$P2_1'/c$ (14.77)	$2'/m$	PT-wP	×
0.244	$Li_2Co(SO_4)_2$	$Pbca$ (61)	$Pb'c'a'$ (61.437)	$m'm'm'$	PT-wP	×
0.245	$Li_{1.5}Fe(SO_4)_2$	$Pbca$ (61)	$P2_1'/c$ (14.77)	$2'/m$	PT-wP	×
0.246	$LiFe(SO_4)_2$	$Pbca$ (61)	$Pb'c'a'$ (61.437)	$m'm'm'$	PT-wP	×
0.247	$Nd_2NiO_{4.11}$	$P4_2/ncm$ (138)	$P4_2/nc'm'$ (138.525)	$4/mm'm'$	×	✓
0.248	$TbPt_{0.8}Cu_{0.2}$	$Pnma$ (62)	$Pn'm'a$ (62.446)	$m'm'm$	×	✓
0.249	$NdNi_{0.6}Cu_{0.4}$	$Pnma$ (62)	$Pnm'a'$ (62.447)	$m'm'm$	×	✓
0.250	$(NH_2(CH_3)_2)(FeCl_3(H_2O))$	$P\bar{3}c1$ (163)	$C2'/c'$ (15.89)	$2'/m'$	×	✓
0.251	$(NH_2(CH_3)_2)(FeMnCl_6)$	$P\bar{3}c1$ (163)	$C2'/c'$ (15.89)	$2'/m'$	×	✓
0.252	$Cs_2FeCl_5.D_2O$	$C2/c$ (15)	$C2'/c$ (15.87)	$2'/m$	PT-wP	×
0.253	$Cs_2FeCl_5.D_2O$	$C2/c$ (15)	$C2$ (5.13)	2	O-wP	✓
0.254	$[C(ND_2)_3]Cu(DCOO)_3$	$Pna2_1$ (33)	$Pna2_1$ (33.144)	$mm2$	O-woP	×
0.255	$[C(ND_2)_3]Cu(DCOO)_3$	$Pna2_1$ (33)	$Pn'a'2_1$ (33.148)	$m'm'2$	BW-woP	✓
0.256	$[C(ND_2)_3]Mn(DCOO)_3$	$Pnna$ (52)	$Pn'n'a$ (52.310)	$m'm'm$	×	✓
0.257	$[C(ND_2)_3]Co(DCOO)_3$	$Pnna$ (52)	$Pn'na'$ (52.312)	$m'm'm$	×	✓
0.258	$Li_3Fe_2(PO_4)_3$	$P2_1/n$ (14)	$P2_1'/c'$ (14.79)	$2'/m'$	×	✓
0.259	$Li_3Fe_2(PO_4)_3$	$R\bar{3}$ (148)	$R\bar{3}$ (148.17)	$\bar{3}$	×	✓

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BCS-ID	Formula	Parent	MSG	MPG	SHG type	LMO
0.260	$CuFePO_5$	$Pnma$ (62)	$Pnma$ (62.441)	mmm	×	×
0.261	$NiFePO_5$	$Pnma$ (62)	$Pnma$ (62.441)	mmm	×	×
0.262	$CoFePO_5$	$Pnma$ (62)	$Pnm'a'$ (62.447)	$m'm'm$	×	✓
0.263	Fe_2PO_5	$Pnma$ (62)	$Pnma$ (62.441)	mmm	×	×
0.264	$Fe_3(PO_4)_2$	$P2_1/c$ (14)	$P2_1/c'$ (14.78)	$2/m'$	PT-wP	×
0.265	$Mn_3(Co_{0.61}Mn_{0.39})N$	$Pm\bar{3}m$ (221)	$R\bar{3}$ (148.17)	$\bar{3}$	×	✓
0.266	$Na_2BaCo(VO_4)_2$	$P\bar{3}m1$ (164)	$P\bar{3}m'1$ (164.89)	$\bar{3}m'$	×	✓
0.267	$YbMnBi_2$	$P4/nmm$ (129)	$P4'/n'm'm$ (129.416)	$4'/m'm'm$	PT-wP	×
0.268	Tb_2MnNiO_6	$P2_1/c$ (14)	$P2_1'$ (4.9)	$2'$	BW-wP	✓
0.269	Tb_2MnNiO_6	$P2_1/c$ (14)	$P2_1'/c'$ (14.79)	$2'/m'$	×	✓
0.270	Tb_2MnNiO_6	$P2_1/c$ (14)	$P2_1'/c'$ (14.79)	$2'/m'$	×	✓
0.271	Tb_2MnNiO_6	$P2_1/c$ (14)	$P2_1'/c'$ (14.79)	$2'/m'$	×	✓
0.272	Tb_2MnNiO_6	$P2_1/c$ (14)	$P2_1/c$ (14.75)	$2/m$	×	✓
0.273	Mn_3ZnN	$Pm\bar{3}m$ (221)	$R\bar{3}m$ (166.97)	$\bar{3}m$	×	×
0.274	Mn_4N	$Pm\bar{3}m$ (221)	$R\bar{3}m'$ (166.101)	$\bar{3}m'$	×	✓
0.275	Mn_3AlN	$Pm\bar{3}m$ (221)	$R\bar{3}m'$ (166.101)	$\bar{3}m'$	×	✓
0.276	Mn_3AlN	$Pm\bar{3}m$ (221)	$Cmm'm'$ (65.486)	$m'm'm$	×	✓
0.277	$MgMnO_3$	$R\bar{3}$ (148)	$R\bar{3}'$ (148.19)	$\bar{3}'$	PT-wP	×
0.278	$Cu_{0.82}Mn_{1.18}As$	$P\bar{6}$ (174)	$P\bar{6}'$ (174.135)	$\bar{6}'$	BW-woP	×
0.279	Mn_3As	$P6_3/mmc$ (194)	$Cmc'm'$ (63.463)	$m'm'm$	×	✓
0.280	Mn_3As	$P6_3/mmc$ (194)	$Cm'cm'$ (63.464)	$m'm'm$	×	✓
0.281	$Co_2V_2O_7$	$P2_1/c$ (14)	$P2_1/c'$ (14.78)	$2/m'$	PT-wP	×
0.282	$U_{14}Au_51$	$P6/m$ (175)	$P6'/m$ (175.139)	$6'/m$	PT-wP	×
0.283	$U_{14}Au_51$	$P6/m$ (175)	$P6/m'$ (175.140)	$6/m'$	PT-wP	×
0.284	$KOsO_4$	$I4_1/a$ (88)	$I4_1'/a'$ (88.85)	$4'/m'$	PT-wP	×
0.285	$KRuO_4$	$I4_1/a$ (88)	$I4_1'/a'$ (88.85)	$4'/m'$	PT-wP	×
0.286	Mn_5Ge_3	$P6_3/mcm$ (193)	$P6_3/mc'm'$ (193.260)	$6/mm'm'$	×	✓
0.287	$SrCo(VO_4)(OH)$	$P2_12_12_1$ (19)	$P2_12_12_1$ (19.25)	222	O-woP	×
0.288	$NdMnO_3$	$Pnma$ (62)	$Pn'ma'$ (62.448)	$m'm'm$	×	✓
0.289	$NdMnO_3$	$Pnma$ (62)	$Pn'ma'$ (62.448)	$m'm'm$	×	✓
0.290	$CeCu_2$	$Imma$ (74)	$Im'm'a'$ (74.560)	$m'm'm'$	PT-wP	×
0.291	Tl_2NiMnO_6	$P2_1/c$ (14)	$P2_1/c$ (14.75)	$2/m$	×	✓
0.292	$NiTe_2O_5$	$Pnma$ (62)	$Pnma$ (62.441)	mmm	×	×
0.293	$(Tm_{0.7}Mn_{0.3})MnO_3$	$Pnma$ (62)	$Pnm'a'$ (62.447)	$m'm'm$	×	✓
0.294	$Cu_4(OD)_6FBr$	$Pnma$ (62)	$Pn'm'a$ (62.446)	$m'm'm$	×	✓
0.295	$Cu_2(OD)_3Cl$	$P2_1/c$ (14)	$P2_1/c$ (14.75)	$2/m$	×	✓
0.296	$Cu_2(OD)_3Cl$	$P2_1/c$ (14)	$P2_1/c$ (14.75)	$2/m$	×	✓
0.297	$NaCrGe_2O_6$	$C2/c$ (15)	$C2'/c'$ (15.89)	$2'/m'$	×	✓
0.298	$Na_2BaFe(VO_4)_2$	$C2/c$ (15)	$C2'/c'$ (15.89)	$2'/m'$	×	✓
0.299	Fe_2O_3	$Pna2_1$ (33)	$Pna'2_1'$ (33.147)	$m'm2'$	BW-woP	✓
0.300	Fe_2O_3	$Pna2_1$ (33)	$Pna'2_1'$ (33.147)	$m'm2'$	BW-woP	✓
0.301	Sr_2CoTeO_6	$P2_1/n$ (14)	$P2_1/c$ (14.75)	$2/m$	×	✓
0.302	$Sr_2Co_{0.9}Mg_{0.1}TeO_6$	$P2_1/n$ (14)	$P2_1/c$ (14.75)	$2/m$	×	✓
0.303	$BaCrF_5$	$P2_12_12_1$ (19)	$P2_1'2_1'2_1$ (19.27)	$2'2'2$	BW-woP	✓
0.304	$Pr_{0.5}Sr_{0.5}CoO_3$	$Imma$ (74)	$Im'm'a$ (74.558)	$m'm'm$	×	✓
0.305	$Pr_{0.5}Sr_{0.5}CoO_3$	$I4/mcm$ (140)	$Fm'm'm$ (69.524)	$m'm'm$	×	✓
0.306	$GaFeO_3$	$R3c$ (161)	Cc' (9.39)	m'	BW-woP	✓
0.307	$ScCrO_3$	$Pnma$ (62)	$Pnma$ (62.441)	mmm	×	×
0.308	$InCrO_3$	$Pnma$ (62)	$Pnma$ (62.441)	mmm	×	×
0.309	$TlCrO_3$	$Pnma$ (62)	$Pnma$ (62.441)	mmm	×	×
0.310	$NaMnFeF_6$	$P321$ (150)	$P32'1$ (150.27)	$32'$	BW-woP	✓
0.311	$CoGeO_3$	$Pbca$ (61)	$Pb'ca$ (61.435)	$m'mm$	PT-wP	×
0.312	$MnGeO_3$	$C2/c$ (15)	$C2'/c$ (15.87)	$2'/m$	PT-wP	×
0.313	$MnGeO_3$	$Pbca$ (61)	$Pb'ca$ (61.435)	$m'mm$	PT-wP	×
0.314	$ZrCo_2Ge_4O_{12}$	$P4/nbm$ (125)	$Pb'an'$ (50.282)	$m'm'm$	×	✓
0.315	$ZrMn_2Ge_4O_{12}$	$P4/nbm$ (125)	$P4'/nbm'$ (125.367)	$4'/mm'm$	×	×

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BCS-ID	Formula	Parent	MSG	MPG	SHG type	LMO
0.316	$DyCrWO_6$	$Pna2_1$ (33)	$P2_1$ (4.7)	2	O-woP	✓
0.317	Ho_2CoMnO_6	$P2_1/c$ (14)	$P2_1'/c'$ (14.79)	$2'/m'$	×	✓
0.318	Tm_2CoMnO_6	$P2_1/c$ (14)	$P2_1'/c'$ (14.79)	$2'/m'$	×	✓
0.319	Tm_2CoMnO_6	$P2_1/c$ (14)	$P2_1'/c'$ (14.79)	$2'/m'$	×	✓
0.320	U_2Pd_2In	$P4/mbm$ (127)	$P4'/m'bm'$ (127.394)	$4'/m'm'm$	PT-wP	×
0.321	U_2Pd_2Sn	$P4/mbm$ (127)	$P4'/m'bm'$ (127.394)	$4'/m'm'm$	PT-wP	×
0.322	$Cu_{1.94}Mn_{1.06}BO_5$	$P2_1/c$ (14)	$P2_1'/c'$ (14.79)	$2'/m'$	×	✓
0.323	$LaCrO_3$	$Pnma$ (62)	$Pnma$ (62.441)	mmm	×	×
0.324	$CdYb_2S_4$	$Fd\bar{3}m$ (227)	$I4_1/amd$ (141.551)	$4/mmm$	×	×
0.325	$CdYb_2Se_4$	$Fd\bar{3}m$ (227)	$I4_1/amd$ (141.551)	$4/mmm$	×	×
0.326	$Nd_2Sn_2O_7$	$Fd\bar{3}m$ (227)	$Fd\bar{3}m'$ (227.131)	$m\bar{3}m'$	×	×
0.327	$CsMnF_4$	$P4/nmm$ (129)	$Pmm'n'$ (59.410)	$m'm'm$	×	✓
0.328	$KMnF_4$	$P2_1/a$ (14)	$P2_1'/c'$ (14.79)	$2'/m'$	×	✓
0.329	$RbMnF_4$	$P2_1/a$ (14)	$P\bar{1}$ (2.4)	$\bar{1}$	×	✓
0.330	$ErGe_3$	$Cmcm$ (63)	$P2_1/m'$ (11.53)	$2/m'$	PT-wP	×
0.331	$Fe_2Mo_3O_8$	$P6_3mc$ (186)	$P6_3'm'c$ (186.205)	$6'mm'$	BW-woP	×
0.332	$Co_2Mo_3O_8$	$P6_3mc$ (186)	$P6_3'm'c$ (186.205)	$6'mm'$	BW-woP	×
0.333	$Mn_2Mo_3O_8$	$P6_3mc$ (186)	$P6_3m'c'$ (186.207)	$6m'm'$	BW-woP	✓
0.334	CoF_3	$R\bar{3}c$ (167)	$R\bar{3}c$ (167.103)	$\bar{3}m$	×	×
0.335	FeF_3	$R\bar{3}c$ (167)	$C2'/c'$ (15.89)	$2'/m'$	×	✓
0.336	$NdFeO_3$	$Pnma$ (62)	$Pn'ma'$ (62.448)	$m'm'm$	×	✓
0.337	$NdFeO_3$	$Pnma$ (62)	$P2_1'/c'$ (14.79)	$2'/m'$	×	✓
0.338	$Co_2Mo_3O_8$	$P6_3mc$ (186)	$P6_3'm'c$ (186.205)	$6'mm'$	BW-woP	×
0.339	$Nd_2Hf_2O_7$	$Fd\bar{3}m$ (227)	$Fd\bar{3}m'$ (227.131)	$m\bar{3}m'$	×	×
0.340	$Nd_2Zr_2O_7$	$Fd\bar{3}m$ (227)	$Fd\bar{3}m'$ (227.131)	$m\bar{3}m'$	×	×
0.341	$DyGe_{1.75}$	$Cmmm$ (65)	$Cm'mm$ (65.483)	$m'mm$	PT-wP	×
0.342	Tb_3Ge_5	$Fdd2$ (43)	$Fdd2$ (43.224)	$mm2$	O-woP	×
0.343	$TbGe_2$	$Cmmm$ (65)	$Cm'mm$ (65.483)	$m'mm$	PT-wP	×
0.344	$ErGe_{1.83}$	$Cmc2_1$ (36)	$Cmc2_1$ (36.172)	$mm2$	O-woP	×
0.345	Tb_2C_3	$I\bar{4}3d$ (220)	$Fd'd2'$ (43.226)	$m'm2'$	BW-woP	✓
0.346	Tb_2ReC_2	$Pnma$ (62)	$Pnma'$ (62.445)	$m'mm$	PT-wP	×
0.347	Er_2ReC_2	$Pnma$ (62)	$P2_1'/c$ (14.77)	$2'/m$	PT-wP	×
0.348	Bi_2CuO_4	$P4/ncc$ (130)	$P4/n'c'c'$ (130.431)	$4/m'm'm'$	PT-wP	×
0.349	Nd_2NiO_4	$P4_2/ncm$ (138)	$P4_2/nc'm'$ (138.525)	$4/mm'm'$	×	✓
0.350	$TbAlO_3$	$Pbnm$ (62)	$Pn'm'a'$ (62.449)	$m'm'm'$	PT-wP	×
0.351	$TbFeO_3$	$Pbnm$ (62)	$Pn'ma'$ (62.448)	$m'm'm$	×	✓
0.352	$TbFeO_3$	$Pbnm$ (62)	$Pn'm'a$ (62.446)	$m'm'm$	×	✓
0.353	$TbFeO_3$	$Pbnm$ (62)	$P2_1'2_1'2_1$ (19.27)	$2'2'2$	BW-wP	✓
0.354	$TbCrO_3$	$Pbnm$ (62)	$Pn'm'a$ (62.446)	$m'm'm$	×	✓
0.355	$Mn_{2.85}Ga_{1.15}$	$P6_3/mmc$ (194)	$P6_3'/m'm'c$ (194.268)	$6'/m'mm'$	×	×
0.356	$Mn_{2.85}Ga_{1.15}$	$I4/mmm$ (139)	$I4/mm'm'$ (139.537)	$4/mm'm'$	×	✓
0.357	$CaFe_5O_7$	$P2_1/m$ (11)	$P2_1/m$ (11.50)	$2/m$	×	✓
0.358	$CaFe_5O_7$	$P2_1/m$ (11)	$P2_1/m'$ (11.54)	$2'/m'$	×	✓
0.359	Mn_2ScSbO_6	$R3$ (146)	$P1$ (1.1)	1	O-woP	✓
0.360	Mn_2ScSbO_6	$P2_1/n$ (14)	$P2_1/c$ (14.75)	$2/m$	×	✓
0.361	Sr_3LiRuO_6	$R\bar{3}c$ (167)	$C2'/c'$ (15.89)	$2'/m'$	×	✓
0.362	$RbFeCl_5(D_2O)$	$Pnma$ (62)	$Pn'm'a'$ (62.449)	$m'm'm'$	PT-wP	×
0.363	$KFeCl_5(D_2O)$	$Pnma$ (62)	$Pn'm'a'$ (62.449)	$m'm'm'$	PT-wP	×
0.364	$SrCr_2As_2$	$I4/mmm$ (139)	$I4'/m'm'm$ (139.536)	$4'/m'm'm$	PT-wP	×
0.365	$BaCr_2As_2$	$I4/mmm$ (139)	$I4'/m'm'm$ (139.536)	$4'/m'm'm$	PT-wP	×
0.366	$BaCrFeAs_2$	$I4/mmm$ (139)	$I4'/m'm'm$ (139.536)	$4'/m'm'm$	PT-wP	×
0.367	$EuCr_2As_2$	$I4/mmm$ (139)	$I\bar{4}m'2'$ (119.319)	$\bar{4}2'm'$	BW-wP	✓
0.368	$(CH_3NH_3)(Co(COOH)_3$	$Pnma$ (62)	$Pn'ma'$ (62.448)	$m'm'm$	×	✓
0.369	$(CH_3NH_3)(Co(COOH)_3$	$P2_1/n$ (14)	$P2_1'/c'$ (14.79)	$2'/m'$	×	✓

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BCS-ID	Formula	Parent	MSG	MPG	SHG type	LMO
0.370	$NdMnO_3$	$Pnma$ (62)	$Pn'ma'$ (62.448)	$m'm'm$	×	✓
0.371	$NdMnO_3$	$Pnma$ (62)	$Pn'ma'$ (62.448)	$m'm'm$	×	✓
0.372	$DyCrO_4$	$I4_1/a$ (88)	$C2'/c$ (15.87)	$2'/m$	PT-wP	×
0.373	$La_{0.75}Bi_{0.25}Fe_{0.5}Cr_{0.5}O_3$	$Pnma$ (62)	$Pnma$ (62.441)	mmm	×	×
0.374	YNi_4Si	$Cmmm$ (65)	$Cmm'm'$ (65.486)	$m'm'm$	×	✓
0.375	La_2CoIrO_6	$P2_1/n$ (14)	$P2_1/c$ (14.75)	$2/m$	×	✓
0.376	$LaCaFeO_4$	$Cmce$ (64)	$Cm'c'a$ (64.474)	$m'm'm$	×	✓
0.377	Mn_3Ge	$P6_3/mmc$ (194)	$Cm'cm'$ (63.464)	$m'm'm$	×	✓
0.378	UBi_2	$P4/nmm$ (129)	$P4/n'm'm'$ (129.419)	$4/m'm'm'$	PT-wP	×
0.379	$SmFeO_3$	$Pbnm$ (62)	$Pn'm'a$ (62.446)	$m'm'm$	×	✓
0.380	$SmFeO_3$	$Pnma$ (62)	$Pn'ma'$ (62.448)	$m'm'm$	×	✓
0.381	$Co_6(OH)_3(TeO_3)_4(PO_4)_3$	$P6_3/m$ (176)	$P6_3'mc'$ (186.206)	$6'mm'$	BW-woP	×
0.382	$LiMnPO_4$	$Pnma$ (62)	$Pn'm'a'$ (62.449)	$m'm'm'$	PT-wP	×
0.383	$LiCoPO_4$	$Pnma$ (62)	$Pnma'$ (62.445)	$m'mm$	PT-wP	×
0.384	$LiCoPO_4$	$Pnma$ (62)	$P2_1'/c$ (14.77)	$2'/m$	PT-wP	×
0.385	$LiCoPO_4$	$Pnma$ (62)	$P2_1/c'$ (14.78)	$2/m'$	PT-wP	×
0.386	Fe_3BO_5	$Pnma$ (62)	$Pnm'a$ (62.444)	$m'mm$	PT-wP	×
0.387	Fe_3BO_5	$Pnma$ (62)	$Pm'c2_1'$ (26.68)	$m'm2'$	BW-wP	✓
0.388	$Co_3Al_2Si_3O_{12}$	$Ia\bar{3}d$ (230)	$I4_1/a'cd$ (142.563)	$4/m'mm$	PT-wP	×
0.389	$Fe_{1.5}Mn_{1.5}BO_5$	$Pbam$ (55)	$Pbam$ (55.353)	mmm	×	×
0.390	$Y_2SrCu_{0.6}Co_{1.4}O_{6.5}$	$Ibam$ (72)	$Ib'a'm$ (72.543)	$m'm'm$	×	✓
0.391	$Y_2SrCu_{0.6}Co_{1.4}O_{6.5}$	$Ibam$ (72)	$Ib'a'm$ (72.543)	$m'm'm$	×	✓
0.392	$Fe_3(PO_4)_2(OH)_2$	$P2_1/c$ (14)	$P2_1/c$ (14.75)	$2/m$	×	✓
0.393	$Cu_4(OH)_6FBr$	$P6_3/m$ (176)	$P2_1'/m'$ (11.54)	$2'/m'$	×	✓
0.394	$Cu_2CdB_2O_6$	$P2_1/c$ (14)	$P2_1/c'$ (14.78)	$2/m'$	PT-wP	×
0.395	$MnPtGa$	$P6_3/mmc$ (194)	$Cm'c'm$ (63.462)	$m'm'm$	×	✓
0.396	$MnPtGa$	$P6_3/mmc$ (194)	$Cm'c'm$ (63.462)	$m'm'm$	×	✓
0.397	$Mn_3Si_2Te_6$	$P\bar{3}1c$ (163)	$C2'/c'$ (15.89)	$2'/m'$	×	✓
0.398	Ca_2RuO_4	$Pbca$ (61)	$Pbca$ (61.433)	mmm	×	×
0.399	$FeOOH$	$Pbnm$ (62)	$Pnma'$ (62.445)	$m'mm$	PT-wP	×
0.400	$Sr_2Fe_{1.9}Co_{0.1}O_{5.5}$	$Cmmm$ (65)	$Cm'm'm'$ (65.487)	$m'm'm'$	PT-wP	×
0.401	$Sr_4Fe_4O_{11}$	$Cmmm$ (65)	$Cm'm'm'$ (65.487)	$m'm'm'$	PT-wP	×
0.402	$Sr_4Fe_4O_{11}$	$Cmmm$ (65)	$Cmm'm'$ (65.486)	$m'm'm$	×	✓
0.403	$NdCo_2$	$Fd\bar{3}m$ (227)	$Imm'a'$ (74.559)	$m'm'm$	×	✓
0.404	Sr_3NaRuO_6	$R\bar{3}c$ (167)	$C2'/c'$ (15.89)	$2'/m'$	×	✓
0.405	$CsCoF_4$	$I\bar{4}c2$ (120)	$I\bar{4}'$ (82.41)	$\bar{4}'$	BW-woP	×
0.406	$GdNiSi_3$	$Cmmm$ (65)	$Cmmm'$ (65.484)	$m'mm$	PT-wP	×
0.407	$NdSi$	$Pnma$ (62)	$Pn'm'a$ (62.446)	$m'm'm$	×	✓
0.408	$PrSi$	$Pnma$ (62)	$Pnm'a'$ (62.447)	$m'm'm$	×	✓
0.409	$TmNi$	$Pnma$ (62)	$Pn'm'a$ (62.446)	$m'm'm$	×	✓
0.410	$GdAlO_3$	$Pbnm$ (62)	$Pn'm'a'$ (62.449)	$m'm'm'$	PT-wP	×
0.411	Tb_5Ge_4	$Pnma$ (62)	$Pnm'a$ (62.444)	$m'mm$	PT-wP	×
0.412	Tb_5Ge_4	$Pnma$ (62)	$Pnm'a$ (62.444)	$m'mm$	PT-wP	×
0.413	$UGeSe$	$I4/mmm$ (139)	$I4/m'm'm'$ (139.539)	$4/m'm'm'$	PT-wP	×
0.414	$AlFe_2B_2$	$Cmmm$ (65)	$Cmm'm'$ (65.486)	$m'm'm$	×	✓
0.415	$EuFe_2P_2$	$I4/mmm$ (139)	$C2'/m'$ (12.62)	$2'/m'$	×	✓
0.416	$LaCrO_3$	$R\bar{3}c$ (167)	$R\bar{3}c$ (167.103)	$\bar{3}m$	×	×
0.417	$LaCrO_3$	$Pnma$ (62)	$Pn'ma'$ (62.448)	$m'm'm$	×	✓
0.418	$K_{0.8}Fe_{1.8}Se_2$	$I4/m$ (87)	$I4/m'$ (87.78)	$4/m'$	PT-wP	×
0.419	$ErGe_2O_7$	$P4_12_12$ (92)	$P4_1'2_12'$ (92.113)	$4'22'$	BW-woP	×
0.420	Sr_2LuRuO_6	$P2_1/n$ (14)	$P2_1/c$ (14.75)	$2/m$	×	✓
0.421	$EuMnSb_2$	$Pnma$ (62)	$Pn'm'a'$ (62.449)	$m'm'm'$	PT-wP	×
0.422	$EuMnSb_2$	$Pnma$ (62)	$P2_1/m'$ (11.53)	$2/m'$	PT-wP	×
0.423	$EuMnSb_2$	$Pnma$ (62)	$Pn'm'a'$ (62.449)	$m'm'm'$	PT-wP	×
0.424	$EuMnSb_2$	$Pnma$ (62)	$Pn'm'a'$ (62.449)	$m'm'm'$	PT-wP	×
0.425	$Na_2CoP_2O_7$	$Pna2_1$ (33)	$Pn'a2_1'$ (33.146)	$m'm2'$	BW-woP	✓

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BCS-ID	Formula	Parent	MSG	MPG	SHG type	LMO
0.426	$EuMnBi_2$	$I4/mmm$ (139)	$I4'/m'm'm$ (139.536)	$4'/m'm'm$	PT-wP	×
0.427	$Sm_2Ti_2O_7$	$Fd\bar{3}m$ (227)	$Fd\bar{3}m'$ (227.131)	$m\bar{3}m'$	×	×
0.428	$BaMn_2Si_2O_7$	$C2/c$ (15)	$C2/c$ (15.85)	$2/m$	×	✓
0.429	$CaCr_{0.86}Fe_{3.14}As_3$	$Pnma$ (62)	$Pn'ma$ (62.443)	$m'mm$	PT-wP	×
0.430	Yb_3Pt_4	$R\bar{3}$ (148)	$R\bar{3}'$ (148.19)	$\bar{3}'$	PT-wP	×
0.431	CuB_2O_4	$I\bar{4}2d$ (122)	$P1$ (1.1)	1	O-woP	✓
0.432	$KMnF_3$	$Pnma$ (62)	$Pn'ma'$ (62.448)	$m'm'm$	×	✓
0.433	$KMnF_3$	$I4/mcm$ (140)	$I4/mcm$ (140.541)	$4/mmm$	×	×
0.434	K_2ReI_6	$P2_1/n$ (14)	$P2_1/c$ (14.75)	$2/m$	×	✓
0.435	$Pb_5Fe_3TiO_{11}Cl$	$P4/mmm$ (123)	P_Bmma (51.302)	$mmm1'$	×	×
0.436	$TbNi_4Si$	$Cmmm$ (65)	$Cmm'm'$ (65.486)	$m'm'm$	×	✓
0.437	Ho_3NiGe_2	$Pnma$ (62)	$Pnm'a'$ (62.447)	$m'm'm$	×	✓
0.438	Pr_3CoGe_2	$Pnma$ (62)	$Pnm'a'$ (62.447)	$m'm'm$	×	✓
0.439	Tb_3NiGe_2	$Pnma$ (62)	$Pn'ma'$ (62.448)	$m'm'm$	×	✓
0.440	$SrCuTe_2O_6$	$P4_132$ (213)	$P4_132$ (213.63)	432	×	×
0.441	$Fe_4Nb_2O_9$	$P\bar{3}c1$ (165)	$C2/c'$ (15.88)	$2/m'$	PT-wP	×
0.442	$Fe_4Nb_2O_9$	$C2/c$ (15)	$C2/c'$ (15.88)	$2/m'$	PT-wP	×
0.443	$Fe_4Nb_2O_9$	$P\bar{3}c1$ (165)	$C2/c'$ (15.88)	$2/m'$	PT-wP	×
0.444	$YbCl_3$	$C2/m$ (12)	$C2'/m$ (12.60)	$2'/m$	PT-wP	×
0.445	$MnCoGe$	$Pnma$ (62)	$Pn'm'a$ (62.446)	$m'm'm$	×	✓
0.446	$MnCoGeB_{0.05}$	$P6_3/mmc$ (194)	$Cm'c'm$ (63.462)	$m'm'm$	×	✓
0.447	$MnCoGeB_{0.05}$	$P6_3/mmc$ (194)	$P6_3/mm'c'$ (194.270)	$6/mm'm'$	×	✓
0.448	Ce_4Ge_3	$I\bar{4}3d$ (220)	$I\bar{4}2d$ (122.333)	$\bar{4}2m$	O-woP	×
0.449	Tb_2Pt	$Pnma$ (62)	$P2_1'/m'$ (11.54)	$2'/m'$	×	✓
0.450	Nd_5Ge_4	$Pnma$ (62)	$Pnm'a'$ (62.447)	$m'm'm$	×	✓
0.451	$DyRuAsO$	$Pmmn$ (59)	$Pm'mn$ (59.407)	$m'mm$	PT-wP	×
0.452	$TbRuAsO$	$P4/nmm$ (129)	$Pm'mn$ (59.407)	$m'mm$	PT-wP	×
0.453	$DyCoSi_2$	$Cmcm$ (63)	$Cm'cm$ (63.459)	$m'mm$	PT-wP	×
0.454	$PrScSb$	$I4/mmm$ (139)	$P-I4/mnc$ (128.410)	$4/mmm1'$	×	×
0.455	$RbFeO_2$	$Pbca$ (61)	$Pb'c'a'$ (61.437)	$m'm'm'$	PT-wP	×
0.456	$RbFeO_2$	$Fd\bar{3}m$ (227)	$I4_1'/a'm'd$ (141.556)	$4'/m'm'm$	PT-wP	×
0.457	$CsFeO_2$	$Pbca$ (61)	$Pb'c'a'$ (61.437)	$m'm'm'$	PT-wP	×
0.458	$CsFeO_2$	$Fd\bar{3}m$ (227)	$I4_1'/a'm'd$ (141.556)	$4'/m'm'm$	PT-wP	×
0.459	$KFeO_2$	$Pbca$ (61)	$Pb'ca$ (61.435)	$m'mm$	PT-wP	×
0.460	$KFeO_2$	$Pbca$ (61)	$Pb'ca$ (61.435)	$m'mm$	PT-wP	×
0.461	$CoRh_2O_4$	$Fd\bar{3}m$ (227)	$I4_1'/a'm'd$ (141.556)	$4'/m'm'm$	PT-wP	×
0.462	$MnAl_2O_4$	$Fd\bar{3}m$ (227)	$I4_1'/a'm'd$ (141.556)	$4'/m'm'm$	PT-wP	×
0.463	Co_3O_4	$Fd\bar{3}m$ (227)	$I4_1'/a'm'd$ (141.556)	$4'/m'm'm$	PT-wP	×
0.464	$BaMn_2P_2$	$I4/mmm$ (139)	$I4'/m'm'm$ (139.536)	$4'/m'm'm$	PT-wP	×
0.465	$HoCr_2Si_2$	$I4/mmm$ (139)	$I4'/m'm'm$ (139.536)	$4'/m'm'm$	PT-wP	×
0.466	$ThCr_2Si_2$	$I4/mmm$ (139)	$Im'mm$ (71.535)	$m'mm$	PT-wP	×
0.467	$TbPO_4$	$I4_1/amd$ (141)	$I4_1'/a'm'd$ (141.556)	$4'/m'm'm$	PT-wP	×
0.468	ErB_4	$P4/mbm$ (127)	$Pb'am$ (55.355)	$m'mm$	PT-wP	×
0.469	TbB_4	$P4/mbm$ (127)	$Pb'a'm'$ (55.359)	$m'm'm'$	PT-wP	×
0.470	$BaMn_2Sb_2$	$I4/mmm$ (139)	$I4'/m'm'm$ (139.536)	$4'/m'm'm$	PT-wP	×
0.471	$Ba_2Mn_3Sb_2O_2$	$I4/mmm$ (139)	$I4'/m'm'm$ (139.536)	$4'/m'm'm$	PT-wP	×
0.472	$LaMn_2Si_2$	$I4/mmm$ (139)	$I4'/m'm'm$ (139.536)	$4'/m'm'm$	PT-wP	×
0.473	$LaMn_2Si_2$	$I4/mmm$ (139)	$Im'm2'$ (44.231)	$m'm2'$	BW-wP	✓
0.474	$EuMn_2Ge_2$	$I4/mmm$ (139)	$I4'/m'm'm$ (139.536)	$4'/m'm'm$	PT-wP	×

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BCS-ID	Formula	Parent	MSG	MPG	SHG type	LMO
0.475	Sr_2TbIrO_6	$P2_1/n$ (14)	$P2_1/c$ (14.75)	$2/m$	×	✓
0.476	$Cs_2[FeCl_5(H_2O)]$	$I2/c$ (15)	$C2'/c$ (15.87)	$2'/m$	PT-wP	×
0.477	$Mn_4Ta_2O_9$	$P\bar{3}c1$ (165)	$P\bar{3}'c'1$ (165.94)	$\bar{3}'m'$	PT-wP	×
0.478	$SmCrO_3$	$Pnma$ (62)	$Pnma$ (62.441)	mmm	×	×
0.479	$SmCrO_3$	$Pnma$ (62)	$Pn'ma'$ (62.448)	$m'm'm$	×	✓
0.480	HoNi	$Pnma$ (62)	$Pnm'a'$ (62.447)	$m'm'm$	×	✓
0.481	HoNi	$Pnma$ (62)	$P2_1'/c'$ (14.79)	$2'/m'$	×	✓
0.482	$SrMn_2As_2$	$P\bar{3}m1$ (164)	$C2'/m$ (12.60)	$2'/m$	PT-wP	×
0.483	$YbMn_2Sb_2$	$P\bar{3}m1$ (164)	$P\bar{1}'$ (2.6)	$\bar{1}'$	PT-wP	×
0.484	U_2N_2S	$P\bar{3}m1$ (164)	$P\bar{3}'m'1$ (164.88)	$\bar{3}'m'$	PT-wP	×
0.485	U_2N_2Se	$P\bar{3}m1$ (164)	$P\bar{3}'m'1$ (164.88)	$\bar{3}'m'$	PT-wP	×
0.486	$ErCr_2Si_2$	$I4/mmm$ (139)	$I4'/m'm'm$ (139.536)	$4'/m'm'm$	PT-wP	×
0.487	$ErCr_2Si_2$	$I4/mmm$ (139)	$Im'm'2$ (44.232)	$m'm'2$	BW-wP	✓
0.488	$YbMnO_3$	$P6_3cm$ (185)	$P6_3'c'm$ (185.199)	$6'mm'$	BW-woP	×
0.489	$YbMnO_3$	$P6_3cm$ (185)	$P6_3'c'm$ (185.199)	$6'mm'$	BW-woP	×
0.490	$YbMnO_3$	$P6_3cm$ (185)	$P6_3c'm'$ (185.201)	$6m'm'$	BW-woP	✓
0.491	NdB_4	$P4/mbm$ (127)	$P4/m'$ (83.46)	$4/m'$	PT-wP	×
0.492	NdB_4	$P4/mbm$ (127)	$P2_1'/c$ (14.77)	$2'/m$	PT-wP	×
0.493	$Ho(Co_{0.667}Ga_{0.333})_2$	$P6_3/mmc$ (194)	$C2'/c'$ (15.89)	$2'/m'$	×	✓
0.494	$Er(Co_{0.667}Ga_{0.333})_2$	$P6_3/mmc$ (194)	$P6_3/mm'c'$ (194.270)	$6/mm'm'$	×	✓
0.495	$LaMn_2Si_2$	$I4/mmm$ (139)	$Im'm2'$ (44.231)	$m'm2'$	BW-wP	✓
0.496	$LaMn_2Si_2$	$I4/mmm$ (139)	$Im'm2'$ (44.231)	$m'm2'$	BW-wP	✓
0.497	$LaMn_2Si_2$	$I4/mmm$ (139)	$Im'm2'$ (44.231)	$m'm2'$	BW-wP	✓
0.498	$LaMn_2Si_2$	$I4/mmm$ (139)	$I4'/m'm'm$ (139.536)	$4'/m'm'm$	PT-wP	×
0.499	UCr_2Si_2C	$P4/mmm$ (123)	$Pm'm'm$ (47.252)	$m'm'm$	×	✓
0.500	$Ca_2FeMn_{0.5}W_{0.5}O_6$	$P2_1/n$ (14)	$P2_1'/c'$ (14.79)	$2'/m'$	×	✓
0.501	$LiFe_2F_6$	$P4_2/mnm$ (136)	$P4_2'/mnm'$ (136.499)	$4'/mm'm$	×	×
0.502	$La_2Ni_{1.19}Os_{0.81}O_6$	$P2_1/c$ (14)	$P2_1'/c'$ (14.79)	$2'/m'$	×	✓
0.503	$K_{1.62}Fe_4O_{6.62}(OH)_{0.38}$	$P\bar{3}1c$ (163)	$P\bar{3}1c$ (163.79)	$\bar{3}m$	×	×
0.504	$NaCrSi_2O_6$	$C2/c$ (15)	$P\bar{1}'$ (2.6)	$\bar{1}'$	PT-wP	×
0.505	$Pb_2VO(PO_4)_2$	$P2_1/a$ (14)	$P2_1/c'$ (14.78)	$2/m'$	PT-wP	×
0.506	$Cs_2Cu_3SnF_{12}$	$P2_1/n$ (14)	$P2_1'/c'$ (14.79)	$2'/m'$	×	✓
0.507	$Mn_4Nb_2O_9$	$P\bar{3}c1$ (165)	$P\bar{3}'c'1$ (165.94)	$\bar{3}'m'$	PT-wP	×
0.508	$FeMnO_3$	$Ia\bar{3}$ (206)	$Ib'c'a$ (73.551)	$m'm'm$	×	✓
0.509	$BaFe_{12}O_{19}$	$P6_3/mmc$ (194)	$P6_3/mm'c'$ (194.270)	$6/mm'm'$	×	✓
0.510	Mn_2NiReO_6	$P2_1/n$ (14)	$P2_1/c$ (14.75)	$2/m$	×	✓
0.511	$Co_4Ta_2O_9$	$P\bar{3}c1$ (165)	$C2'/c$ (15.87)	$2'/m$	PT-wP	×
0.512	Mn_3As_2	$C2/m$ (12)	$C2/m$ (12.58)	$2/m$	×	✓
0.513	$YRuO_3$	$Pnma$ (62)	$Pn'ma'$ (62.448)	$m'm'm$	×	✓
0.514	$CoFe_3O_5$	$Cmcm$ (63)	$Cm'cm'$ (63.464)	$m'm'm$	×	✓
0.515	$CoFe_3O_5$	$Cmcm$ (63)	$P2_1'/m'$ (11.54)	$2'/m'$	×	✓
0.516	$BaMg_2Fe_{16}O_{27}$	$P6_3/mmc$ (194)	$P6_3/mm'c'$ (194.270)	$6/mm'm'$	×	✓
0.517	$BaCo_2Fe_{16}O_{27}$	$P6_3/mmc$ (194)	$P6_3/mm'c'$ (194.270)	$6/mm'm'$	×	✓
0.518	$TbCr_2Si_2$	$I4/mmm$ (139)	$I4'/m'm'm$ (139.536)	$4'/m'm'm$	PT-wP	×
0.519	$HoCr_2Si_2$	$I4/mmm$ (139)	$I4'/m'm'm$ (139.536)	$4'/m'm'm$	PT-wP	×
0.520	$TbCoO_3$	$Pbnm$ (62)	$Pnm'a$ (62.444)	$m'mm$	PT-wP	×
0.521	$DyCoO_3$	$Pbnm$ (62)	$Pn'm'a'$ (62.449)	$m'm'm'$	PT-wP	×
0.522	$La_2O_3FeMnSe_2$	$I4/mmm$ (139)	$Im'm'm$ (71.536)	$m'm'm$	×	✓
0.523	$CaMn_2Sb_2$	$P\bar{3}m1$ (164)	$P\bar{1}'$ (2.6)	$\bar{1}'$	PT-wP	×

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TABLE S1 – continued from previous page

BCS-ID	Formula	Parent	MSG	MPG	SHG type	LMO
0.524	$MnPSe_3$	$R\bar{3}$ (148)	$P\bar{1}'$ (2.6)	$\bar{1}'$	PT-wP	×
0.525	$NaCeO_2$	$I4_1/amd$ (141)	$I4_1'/a'm'd$ (141.556)	$4'/m'm'm$	PT-wP	×
0.526	$Mn_4Ta_2O_9$	$P\bar{3}c1$ (165)	$P\bar{3}'c'1$ (165.94)	$\bar{3}'m'$	PT-wP	×
0.527	$Er_2Si_2O_7$	$C2/m$ (12)	$C2'/m$ (12.60)	$2'/m$	PT-wP	×
0.528	$CrSb$	$P6_3/mmc$ (194)	$P6_3'/m'm'c$ (194.268)	$6'/m'mm'$	×	×
0.529	$Co_4Nb_2O_9$	$P\bar{3}c1$ (165)	$C2/c'$ (15.88)	$2/m'$	PT-wP	×
0.530	$SrCuTe_2O_6$	$P4_132$ (213)	$P4_132$ (213.63)	432	×	×
0.531	$Sr_{0.7}Tb_{0.3}CoO_{2.9}$	$I4/mmm$ (139)	$I4'/mmm'$ (139.535)	$4'/mm'm$	×	×
0.532	$Sr_{0.7}Ho_{0.3}CoO_{2.7}$	$I4/mmm$ (139)	$I4'/mmm'$ (139.535)	$4'/mm'm$	×	×
0.533	$Sr_{0.7}Er_{0.3}CoO_{2.8}$	$I4/mmm$ (139)	$I4'/mmm'$ (139.535)	$4'/mm'm$	×	×
0.534	$Tb_{0.55}Sr_{0.45}MnO_3$	$Pnma$ (62)	$Pnm'a'$ (62.447)	$m'm'm$	×	✓
0.535	$Tb_{0.55}Sr_{0.45}MnO_3$	$Pnma$ (62)	$Pnm'a'$ (62.447)	$m'm'm$	×	✓
0.536	$Tb_{0.55}Sr_{0.45}MnO_3$	$Pnma$ (62)	$Pnm'a'$ (62.447)	$m'm'm$	×	✓
0.537	$CaMn_{0.7}Co_{1.3}ReO_6$	$P4_2/n$ (86)	$P42/n$ (86.67)	$4/m$	×	✓
0.538	$CaMn_{1.2}Ni_{0.8}ReO_6$	$P4_2/n$ (86)	$P42/n$ (86.67)	$4/m$	×	✓
0.539	$Mn_2Fe_{0.8}Mo_{1.2}O_6$	$P2_1/n$ (14)	$P2_1/c$ (14.75)	$2/m$	×	✓
0.540	$Mn_2Fe_{0.8}Mo_{1.2}O_6$	$P2_1/n$ (14)	$P2_1/c$ (14.75)	$2/m$	×	✓
0.541	Mn_2FeReO_6	$P2_1/c$ (14)	$P2_1'/c'$ (14.79)	$2'/m'$	×	✓
0.542	Mn_2FeReO_6	$P2_1/c$ (14)	$P\bar{1}$ (2.4)	$\bar{1}$	×	✓
0.543	Mn_2FeReO_6	$P2_1/c$ (14)	$P\bar{1}$ (2.4)	$\bar{1}$	×	✓
0.544	Mn_2FeReO_6	$P2_1/c$ (14)	$P\bar{1}$ (2.4)	$\bar{1}$	×	✓
0.545	Mn_2FeReO_6	$P2_1/c$ (14)	$P\bar{1}$ (2.4)	$\bar{1}$	×	✓
0.546	Mn_2FeReO_6	$P2_1/c$ (14)	$P2_1'/c'$ (14.79)	$2'/m'$	×	✓
0.547	Mn_2FeReO_6	$P2_1/c$ (14)	$P2_1'/c'$ (14.79)	$2'/m'$	×	✓
0.548	Mn_2FeReO_6	$P2_1/c$ (14)	$P\bar{1}$ (2.4)	$\bar{1}$	×	✓
0.549	Mn_2FeReO_6	$P2_1/c$ (14)	$P\bar{1}$ (2.4)	$\bar{1}$	×	✓
0.550	Mn_3ReO_6	$P2_1/c$ (14)	$P_S\bar{1}$ (2.7)	$\bar{1}1'$	×	×
0.551	Mn_3ReO_6	$P2_1/c$ (14)	$P_S\bar{1}$ (2.7)	$\bar{1}1'$	×	×
0.552	Pb_2MnO_4	$P\bar{4}2_1c$ (114)	$P\bar{4}'2_1c'$ (114.278)	$\bar{4}'2m'$	BW-woP	×
0.553	K_2ReI_6	$P2_1/n$ (14)	$P2_1/c$ (14.75)	$2/m$	×	✓
0.554	Co_2MnSi	$Fm\bar{3}m$ (225)	$I4/mm'm'$ (139.537)	$4/mm'm'$	×	✓
0.555	$Ho_{0.05}Bi_{0.95}FeO_3$	$R3c$ (161)	$R3c$ (161.69)	$3m$	O-woP	×
0.556	$Ho_{0.1}Bi_{0.9}FeO_3$	$R3c$ (161)	$R3c$ (161.69)	$3m$	O-woP	×
0.557	$Ho_{0.15}Bi_{0.85}FeO_3$	$R3c$ (161)	Cc (9.37)	m	O-woP	✓
0.558	$Ho_{0.2}Bi_{0.8}FeO_3$	$R3c$ (161)	Cc (9.37)	m	O-woP	✓
0.559	$Ho_{0.15}Bi_{0.85}FeO_3$	$Pnma$ (62)	$Pn'ma'$ (62.448)	$m'm'm$	×	✓
0.560	$Ho_{0.2}Bi_{0.8}FeO_3$	$Pnma$ (62)	$Pn'ma'$ (62.448)	$m'm'm$	×	✓
0.561	$NdNiGe_2$	$Cmcm$ (63)	$Cm'c'm$ (63.462)	$m'm'm$	×	✓
0.562	$Ce_2Ni_3Ge_5$	$Ibam$ (72)	P_Ibcn (60.432)	$mmm1'$	×	×
0.563	$Ce_2Ni_3Ge_5$	$Ibam$ (72)	P_Iccn (56.376)	$mmm1'$	×	×
0.564	$U_2Rh_3Si_5$	$I2/c$ (15)	P_C2/c (13.74)	$2/m1'$	×	×
0.565	$Ce_2Ni_3Ge_5$	$Ibam$ (72)	P_Ibcn (60.432)	$mmm1'$	×	×
0.566	$TbNiGe_2$	$Cmcm$ (63)	$Cm'cm$ (63.459)	$m'mm$	PT-wP	×
0.567	$HoNi_{0.64}Ge_2$	$Cmcm$ (63)	$Cm'cm$ (63.459)	$m'mm$	PT-wP	×
0.568	$TbNi_{0.4}Ge_2$	$Cmcm$ (63)	$Cm'cm$ (63.459)	$m'mm$	PT-wP	×
0.569	$TbCu_{0.4}Ge_2$	$Cmcm$ (63)	$Cm'cm$ (63.459)	$m'mm$	PT-wP	×
0.570	$Li_{0.5}FeCr_{1.5}O_4$	$Fd\bar{3}m$ (227)	$I4_1/am'd'$ (141.557)	$4/mm'm'$	×	✓
0.571	$CoSO_4$	$Pbnm$ (62)	$Pnma$ (62.441)	mmm	×	×
0.572	Na_2NiCrF_7	$Imma$ (74)	$Im'm'a$ (74.558)	$m'm'm$	×	✓
0.573	Na_2NiCrF_7	$Imma$ (74)	$Im'm'a$ (74.558)	$m'm'm$	×	✓
0.574	$MnFeF_5(H_2O)_2$	$Imm2$ (44)	$C2'$ (5.15)	$2'$	BW-woP	✓
0.575	$ZnFeF_5(H_2O)_2$	$Imm2$ (44)	$Imm2$ (44.229)	$mm2$	O-woP	×
0.576	Cr_2F_5	$C2/c$ (15)	$C2/c$ (15.85)	$2/m$	×	✓
0.577	$BaMnFeF_7$	$P2_1/c$ (14)	$P2_1'/c'$ (14.79)	$2'/m'$	×	✓
0.578	$NaBaFe_2F_9$	$P2_1/c$ (14)	$P2_1/c$ (14.75)	$2/m$	×	✓
0.579	Na_2NiFeF_7	$Imma$ (74)	$Imm'a'$ (74.559)	$m'm'm$	×	✓

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BCS-ID	Formula	Parent	MSG	MPG	SHG type	LMO
0.580	Na_2NiFeF_7	$Imma$ (74)	$Imm'a'$ (74.559)	$m'm'm$	×	✓
0.581	FeF_3	$R\bar{3}c$ (167)	$C2'/c'$ (15.89)	$2'/m'$	×	✓
0.582	$Fe_3F_8(H_2O)_2$	$C2/m$ (12)	$C2'/m'$ (12.62)	$2'/m'$	×	✓
0.583	$Fe_2F_5(H_2O)_2$	$Imma$ (74)	$Imm'a'$ (74.559)	$m'm'm$	×	✓
0.584	$Fe_2F_5(H_2O)_2$	$Imma$ (74)	$C2'/c'$ (15.89)	$2'/m'$	×	✓
0.585	$YbCl_3$	$C2/m$ (12)	$C2'/m$ (12.60)	$2'/m$	PT-wP	×
0.586	$YCrO_3$	$Pbnm$ (62)	$Pn'ma'$ (62.448)	$m'm'm$	×	✓
0.587	$TmCrO_3$	$Pbnm$ (62)	$Pn'ma'$ (62.448)	$m'm'm$	×	✓
0.588	$PrCrO_3$	$Pbnm$ (62)	$Pn'ma'$ (62.448)	$m'm'm$	×	✓
0.589	$NdCrO_3$	$Pbnm$ (62)	$P2_1/m$ (11.50)	$2/m$	×	✓
0.590	$ErCrO_3$	$Pbnm$ (62)	$P2_1/m$ (11.50)	$2/m$	×	✓
0.591	$ErCrO_3$	$Pbnm$ (62)	$Pn'ma'$ (62.448)	$m'm'm$	×	✓
0.592	$DyCrO_3$	$Pbnm$ (62)	$Pn'm'a$ (62.446)	$m'm'm$	×	✓
0.593	UPSe	$P4/nmm$ (129)	$P4/nm'm'$ (129.417)	$4/mm'm'$	×	✓
0.594	UAsS	$P4/nmm$ (129)	$P4/nm'm'$ (129.417)	$4/mm'm'$	×	✓
0.595	UPTe	$I4/mmm$ (139)	$I4/mm'm'$ (139.537)	$4/mm'm'$	×	✓
0.596	UAsTe	$I4/mmm$ (139)	$I4/mm'm'$ (139.537)	$4/mm'm'$	×	✓
0.597	$MnBi_8Te_{13}$	$R\bar{3}m$ (166)	$R\bar{3}m'$ (166.101)	$3m'$	×	✓
0.598	$AlCr_2$	$I4/mmm$ (139)	P_A2_1/c (14.83)	$2/m1'$	×	×
0.599	CaMnSi	$P4/nmm$ (129)	$P4'/n'm'm$ (129.416)	$4'/m'm'm$	PT-wP	×
0.600	CaMnSi	$P4/nmm$ (129)	$P4'/n'm'm$ (129.416)	$4'/m'm'm$	PT-wP	×
0.601	CaMnGe	$P4/nmm$ (129)	$P2_1/m'$ (11.53)	$2/m'$	PT-wP	×
0.602	CaMnGe	$P4/nmm$ (129)	$P2_1/m'$ (11.53)	$2/m'$	PT-wP	×
0.603	$CaMn_2Ge_2$	$I4/mmm$ (139)	$I4'/m'm'm$ (139.536)	$4'/m'm'm$	PT-wP	×
0.604	$CaMn_2Ge_2$	$I4/mmm$ (139)	$I4'/m'm'm$ (139.536)	$4'/m'm'm$	PT-wP	×
0.605	$BaMn_2Ge_2$	$I4/mmm$ (139)	$I4'/m'm'm$ (139.536)	$4'/m'm'm$	PT-wP	×
0.606	$BaMn_2Ge_2$	$I4/mmm$ (139)	$I4'/m'm'm$ (139.536)	$4'/m'm'm$	PT-wP	×
0.607	RuO_2	$P4_2/mnm$ (136)	$P4_2'/mnm'$ (136.499)	$4'/mm'm$	×	×
0.608	$PrMnO_3$	$Pbnm$ (62)	$Pn'ma'$ (62.448)	$m'm'm$	×	✓
0.609	$NdMnO_3$	$Pbnm$ (62)	$P2_1/m$ (11.50)	$2/m$	×	✓
0.610	$Pr_{0.95}K_{0.05}MnO_3$	$Pbnm$ (62)	$Pn'ma'$ (62.448)	$m'm'm$	×	✓
0.611	$BaMnSb_2$	$I4/mmm$ (139)	$I4'/m'm'm$ (139.536)	$4'/m'm'm$	PT-wP	×
0.612	Cu_2OSO_4	$C2/m$ (12)	$C2/m$ (12.58)	$2/m$	×	✓
0.613	$FeCr_2S_4$	$Fd\bar{3}m$ (227)	$I4_1/am'd'$ (141.557)	$4/mm'm'$	×	✓
0.614	$FeCr_2S_4$	$Fd\bar{3}m$ (227)	$I4_1/am'd'$ (141.557)	$4/mm'm'$	×	✓
0.615	$FeCr_2S_4$	$Fd\bar{3}m$ (227)	$I4_1/am'd'$ (141.557)	$4/mm'm'$	×	✓
0.616	HoB_2	$P6/mmm$ (191)	$C2'/m'$ (12.62)	$2'/m'$	×	✓
0.617	KMnSb	$P4/nmm$ (129)	$P4'/n'm'm$ (129.416)	$4'/m'm'm$	PT-wP	×
0.618	KMnBi	$P4/nmm$ (129)	$P4'/n'm'm$ (129.416)	$4'/m'm'm$	PT-wP	×
0.619	LaMnAsO	$P4/nmm$ (129)	$P4'/n'm'm$ (129.416)	$4'/m'm'm$	PT-wP	×
0.620	NdMnAsO	$P4/nmm$ (129)	$P4'/n'm'm$ (129.416)	$4'/m'm'm$	PT-wP	×
0.621	NdMnAsO	$P4/nmm$ (129)	$Pm'mn$ (59.407)	$m'mm$	PT-wP	×
0.622	NdMnAsO	$P4/nmm$ (129)	$Pm'mn$ (59.407)	$m'mm$	PT-wP	×
0.623	NdMnAsO	$P4/nmm$ (129)	$P4'/n'm'm$ (129.416)	$4'/m'm'm$	PT-wP	×
0.624	LaMnAsO	$P4/nmm$ (129)	$P4'/n'm'm$ (129.416)	$4'/m'm'm$	PT-wP	×

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BCS-ID	Formula	Parent	MSG	MPG	SHG type	LMO
0.625	U_2Pd_2In	$P4/mbm$ (127)	$P4'/m'bm'$ (127.394)	$4'/m'm'm$	PT-wP	×
0.626	NaMnP	$P4/nmm$ (129)	$P4'/n'm'm$ (129.416)	$4'/m'm'm$	PT-wP	×
0.627	NaMnP	$P4/nmm$ (129)	$P4'/n'm'm$ (129.416)	$4'/m'm'm$	PT-wP	×
0.628	NaMnP	$P4/nmm$ (129)	$P4'/n'm'm$ (129.416)	$4'/m'm'm$	PT-wP	×
0.629	NaMnAs	$P4/nmm$ (129)	$P4'/n'm'm$ (129.416)	$4'/m'm'm$	PT-wP	×
0.630	NaMnAs	$P4/nmm$ (129)	$P4'/n'm'm$ (129.416)	$4'/m'm'm$	PT-wP	×
0.631	NaMnSb	$P4/nmm$ (129)	$P4'/n'm'm$ (129.416)	$4'/m'm'm$	PT-wP	×
0.632	NaMnSb	$P4/nmm$ (129)	$P4'/n'm'm$ (129.416)	$4'/m'm'm$	PT-wP	×
0.633	$KFeS_2$	$C2/c$ (15)	$C2'/c$ (15.87)	$2'/m$	PT-wP	×
0.634	NaMnBi	$P4/nmm$ (129)	$P4'/n'm'm$ (129.416)	$4'/m'm'm$	PT-wP	×
0.635	NaMnBi	$P4/nmm$ (129)	$P4'/n'm'm$ (129.416)	$4'/m'm'm$	PT-wP	×
0.636	$RbFeS_2$	$C2/c$ (15)	$C2'/c$ (15.87)	$2'/m$	PT-wP	×
0.637	$KFeSe_2$	$C2/c$ (15)	$C2/c'$ (15.88)	$2/m'$	PT-wP	×
0.638	$RbFeSe_2$	$C2/c$ (15)	$C2/c'$ (15.88)	$2/m'$	PT-wP	×
0.639	Mn_2Au	$I4/mmm$ (139)	$Im'mm$ (71.535)	$m'mm$	PT-wP	×
0.640	Mn_2Au	$I4/mmm$ (139)	$Im'mm$ (71.535)	$m'mm$	PT-wP	×
0.641	Mn_3Ga	$I4/mmm$ (139)	$C2'/m'$ (12.62)	$2'/m'$	×	✓
0.642	$LaMnO_3$	$Pnma$ (62)	$Pn'ma'$ (62.448)	$m'm'm$	×	✓
0.643	$La_{0.95}Ca_{0.05}MnO_3$	$Pnma$ (62)	$Pn'ma'$ (62.448)	$m'm'm$	×	✓
0.644	$La_{0.95}Ba_{0.05}MnO_3$	$Pnma$ (62)	$Pn'ma'$ (62.448)	$m'm'm$	×	✓
0.645	$La_{0.95}Ba_{0.05}Mn_{0.95}Ti_{0.05}O_3$	$Pnma$ (62)	$Pn'ma'$ (62.448)	$m'm'm$	×	✓
0.646	$La_{0.90}Ba_{0.10}Mn_{0.90}Ti_{0.10}O_3$	$Pnma$ (62)	$Pn'ma'$ (62.448)	$m'm'm$	×	✓
0.647	$La_{0.875}Ba_{0.125}Mn_{0.875}Ti_{0.125}O_3$	$Pnma$ (62)	$Pn'ma'$ (62.448)	$m'm'm$	×	✓
0.648	$(Ho_{0.8}Mn_{0.2})MnO_3$	$Pnma$ (62)	$Pnm'a'$ (62.447)	$m'm'm$	×	✓
0.649	$(Ho_{0.8}Mn_{0.2})MnO_3$	$Pnma$ (62)	$Pnm'a'$ (62.447)	$m'm'm$	×	✓
0.650	$ErSi_2O_7$	$C2/m$ (12)	$C2'/m$ (12.60)	$2'/m$	PT-wP	×
0.651	$Er_3Cu_4Sn_4$	$C2/m$ (12)	C_c2/m (12.63)	$2/m1'$	×	×
0.652	$HoMnO_3$	$P6_3cm$ (185)	$P6_3'cm'$ (185.2)	$6'mm'$	BW-woP	×
0.653	$HoMn_{0.99}Fe_{0.01}O_3$	$P6_3cm$ (185)	$P6_3'cm'$ (185.2)	$6'mm'$	BW-woP	×
0.654	$HoMn_{0.95}Fe_{0.05}O_3$	$P6_3cm$ (185)	$P6_3'cm'$ (185.2)	$6'mm'$	BW-woP	×
0.655	$HoMn_{0.9}Fe_{0.1}O_3$	$P6_3cm$ (185)	$P6_3'cm'$ (185.2)	$6'mm'$	BW-woP	×
0.656	$NdMn_2Ge_2$	$I4/mmm$ (139)	$Im'm2'$ (44.231)	$m'm2'$	BW-wP	✓
0.657	$PrMn_2Ge_2$	$I4/mmm$ (139)	$Im'm2'$ (44.231)	$m'm2'$	BW-wP	✓
0.658	$BaCuTe_2O_6$	$P4_132$ (213)	$P4_1'32'$ (213.65)	$4'32'$	BW-woP	×
0.659	$NdMn_{0.8}Fe_{0.2}O_3$	$Pnma$ (62)	$Pn'ma'$ (62.448)	$m'm'm$	×	✓
0.660	$NdMn_{0.8}Fe_{0.2}O_3$	$Pnma$ (62)	$Pn'ma'$ (62.448)	$m'm'm$	×	✓
0.661	$(Lu_{0.6}Mn_{0.4})MnO_3$	$Pnma$ (62)	$Pnm'a'$ (62.447)	$m'm'm$	×	✓
0.662	Mn_3Sn_2	$Pnma$ (62)	$Pn'ma'$ (62.448)	$m'm'm$	×	✓
0.663	Mn_3Sn_2	$Pnma$ (62)	$Pn'ma'$ (62.448)	$m'm'm$	×	✓
0.664	Mn_3Sn_2	$Pnma$ (62)	$P2_1'/c'$ (14.79)	$2'/m'$	×	✓
0.665	CeMnSbO	$P4/nmm$ (129)	$P4'/n'm'm$ (129.416)	$4'/m'm'm$	PT-wP	×
0.666	CeMnSbO	$P4/nmm$ (129)	$Pm'mn$ (59.407)	$m'mm$	PT-wP	×
0.667	LaMnSbO	$P4/nmm$ (129)	$P4'/n'm'm$ (129.416)	$4'/m'm'm$	PT-wP	×
0.668	PrMnSbO	$P4/nmm$ (129)	$Pm'mn$ (59.407)	$m'mm$	PT-wP	×
0.669	Sr_2YbRuO_6	$P112_1/n$ (14)	$P2_1/c$ (14.75)	$2/m$	×	✓
0.670	Sr_2YbRuO_6	$P2_1/n$ (14)	$P2_1/c$ (14.75)	$2/m$	×	✓
0.671	Sr_2TmRuO_6	$P2_1/n$ (14)	$P2_1/c$ (14.75)	$2/m$	×	✓

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BCS-ID	Formula	Parent	MSG	MPG	SHG type	LMO
0.672	$CaCu_3Fe_2Sb_2O_{12}$	$Pn\bar{3}$ (201)	$Pn'n'n$ (48.260)	$m'm'm$	×	✓
0.673	$MnFe_4Si_3$	$P6_3/mcm$ (193)	$P6_3/mc'm'$ (193.260)	$6/mm'm'$	×	✓
0.674	$MnFe_4Si_3$	$P6_3/mcm$ (193)	$P6_3/mc'm'$ (193.260)	$6/mm'm'$	×	✓
0.675	$MnFe_4Si_3$	$P6_3/mcm$ (193)	$P6_3/mc'm'$ (193.260)	$6/mm'm'$	×	✓
0.676	$Nd_{0.95}Sr_{0.05}CrO_3$	P (62)	$Pnma$ (62.441)	mmm	×	×
0.677	$Nd_{0.9}Sr_{0.1}CrO_3$	$Pbnm$ (62)	$Pnma$ (62.441)	mmm	×	×
0.678	$Nd_{0.85}Sr_{0.15}CrO_3$	$Pbnm$ (62)	$Pnma$ (62.441)	mmm	×	×
0.679	$TbCr_{0.5}Mn_{0.5}O_3$	$Pbnm$ (62)	$Pn'ma'$ (62.448)	$m'm'm$	×	✓
0.680	$Bi_{0.8}La_{0.2}Fe_{0.5}Mn_{0.5}O_3$	$Imma$ (74)	$Imm'a'$ (74.559)	$m'm'm$	×	✓
0.681	Ce_4Sb_3	$I\bar{4}3d$ (220)	$I\bar{4}'2d'$ (122.336)	$\bar{4}'2m'$	BW-woP	×
0.682	Ca_2FeOsO_6	$P2_1/n$ (14)	$P2_1'/c'$ (14.79)	$2'/m'$	×	✓
0.683	$SrCaFeOsO_6$	$P2_1/n$ (14)	$P2_1'/c'$ (14.79)	$2'/m'$	×	✓
0.684	TbPt	$Pnma$ (62)	$Pn'm'a$ (62.446)	$m'm'm$	×	✓
0.685	ErPt	$Pnma$ (62)	$Pnm'a'$ (62.447)	$m'm'm$	×	✓
0.686	HoPt	$Pnma$ (62)	$Pnm'a'$ (62.447)	$m'm'm$	×	✓
0.687	DyPt	$Pnma$ (62)	$Pn'm'a$ (62.446)	$m'm'm$	×	✓
0.688	TmPt	$Pnma$ (62)	$Pnm'a'$ (62.447)	$m'm'm$	×	✓
0.689	PrPt	$Cmcm$ (63)	$Cm'c'm$ (63.462)	$m'm'm$	×	✓
0.690	NdPt	$Cmcm$ (63)	$C2'/c'$ (15.89)	$2'/m'$	×	✓
0.691	$CaCo_{1.86}As_2$	$I4/mmm$ (139)	P_I4/nnc (126.386)	$4/mmm1'$	×	×
0.692	Ba_4Ru_3O10	$Cmce$ (64)	$Cm'ca$ (64.471)	$m'mm$	PT-wP	×
0.693	Ba_4Ru_3O10	$Cmce$ (64)	$Cmc'a$ (64.472)	$m'mm$	PT-wP	×
0.694	Bi_2CuO_4	$P4/ncc$ (130)	$P4/n'c'c'$ (130.431)	$4/m'm'm'$	PT-wP	×
0.695	Bi_2CuO_4	$P4/ncc$ (130)	$Pc'cn$ (56.367)	$m'mm$	PT-wP	×
0.696	$SmCrO_3$	$Pbnm$ (62)	$Pn'ma'$ (62.448)	$m'm'm$	×	✓
0.697	$SmCrO_3$	$Pbnm$ (62)	$Pn'm'a$ (62.446)	$m'm'm$	×	✓
0.698	$SmCrO_3$	$Pbnm$ (62)	$Pbn'm'$ (62.446)	$m'm'm$	×	✓
0.699	$LiMn_6Sn_6$	$P6/mmm$ (191)	$Cmm'm'$ (65.486)	$m'm'm$	×	✓
0.700	$TbMn_6Sn_6$	$P6/mmm$ (191)	$P6/mm'm'$ (191.240)	$6/mm'm'$	×	✓
0.701	$TbMn_6Sn_6$	$P6/mmm$ (191)	$P6/mm'm'$ (191.240)	$6/mm'm'$	×	✓
0.702	$TbMn_6Sn_6$	$P6/mmm$ (191)	$C2'/m'$ (12.62)	$2'/m'$	×	✓
0.703	$HoMn_6Sn_6$	$P6/mmm$ (191)	$C2'/m'$ (12.62)	$2'/m'$	×	✓
0.704	$HoMn_6Sn_6$	$P6/mmm$ (191)	$C2'/m'$ (12.62)	$2'/m'$	×	✓
0.705	$HoMn_6Sn_6$	$P6/mmm$ (191)	$Cmm'm'$ (65.486)	$m'm'm$	×	✓
0.706	$Tb_2Ir_3Ga_9$	$Cmcm$ (63)	$Cm'cm'$ (63.464)	$m'm'm$	×	✓
0.707	$Tb_2Ir_3Ga_9$	$Cmcm$ (63)	$Cm'cm'$ (63.464)	$m'm'm$	×	✓
0.708	$CrNb_4S_8$	$P6_3/mmc$ (194)	$P6_3'/m'm'c$ (194.268)	$6'/m'mm'$	×	×
0.709	$MnNb_4S_8$	$P6_3/mmc$ (194)	$Cmc'm'$ (63.463)	$m'm'm$	×	✓
0.710	$MnNb_3S_6$	$P6_322$ (182)	$C22'2_1'$ (20.34)	$2'2'2$	BW-woP	✓
0.711	$MnTa_4S_8$	$P6_3/mmc$ (194)	$Cmc'm'$ (63.463)	$m'm'm$	×	✓
0.712	VNb_3S_6	$P6_322$ (182)	$C2'2'2_1$ (20.33)	$2'2'2$	BW-woP	✓
0.713	$NiFe_2O_4$	$Fd\bar{3}m$ (227)	$I4_1/am'd'$ (141.557)	$4/mm'm'$	×	✓
0.714	$Li_2Ni(SO_4)_2$	$P2_1/c$ (14)	$P2_1/c$ (14.75)	$2/m$	×	✓
0.715	$HoCrWO_6$	$Pna2_1$ (33)	$Pna2_1$ (33.144)	$mm2$	O-woP	×
0.716	$HoCrWO_6$	$Pna2_1$ (33)	$Pna2_1$ (33.144)	$mm2$	O-woP	×
0.717	$Pr_{0.5}Sr_{0.4}Ba_{0.1}CoO_3$	$Imma$ (74)	$Im'm'a$ (74.558)	$m'm'm$	×	✓
0.718	$Pr_{0.5}Sr_{0.4}Ba_{0.1}CoO_3$	$I4/mcm$ (140)	$Fm'm'm$ (69.524)	$m'm'm$	×	✓
0.719	$Yb_{0.42}Sc_{0.58}FeO_3$	$P6_3cm$ (185)	$P6_3c'm'$ (185.201)	$6m'm'$	BW-woP	✓
0.720	$Yb_{0.42}Sc_{0.58}FeO_3$	$P6_3cm$ (185)	$P6_3$ (173.129)	6	O-woP	✓
0.721	$Yb_{0.42}Sc_{0.58}FeO_3$	$P6_3cm$ (185)	$P6_3$ (173.129)	6	O-woP	✓
0.722	$Mn_4Nb_2O_9$	Cc (9)	Cc (9.37)	m	O-woP	✓
0.723	$YbCl_3$	$C2/m$ (12)	$C2'/m$ (12.60)	$2'/m$	PT-wP	×

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BCS-ID	Formula	Parent	MSG	MPG	SHG type	LMO
0.724	$BaCoSiO_4$	$P6_3$ (173)	$P6_3$ (173.129)	6	O-woP	✓
0.725	Ce_5TeO_8	$Fd\bar{3}m$ (227)	$I4_1/am'd'$ (141.557)	$4/mm'm'$	×	✓
0.726	$CsMn_2F_6$	$Pnma$ (62)	$Pnm'a'$ (62.447)	$m'm'm$	×	✓
0.727	$CsMn_2F_6$	$Pnma$ (62)	$P2_1/c$ (14.75)	$2/m$	×	✓
0.728	MoP_3SiO_{11}	$R\bar{3}c$ (167)	$C2/c'$ (15.88)	$2/m'$	PT-wP	×
0.729	$ErNi_4B$	$P6/mmm$ (191)	$P6/mm'm'$ (191.240)	$6/mm'm'$	×	✓
0.730	$TbNi_4B$	$P6/mmm$ (191)	$C2'/m'$ (12.62)	$2'/m'$	×	✓
0.731	$HoNi_4B$	$P6/mmm$ (191)	$C2'/m'$ (12.62)	$2'/m'$	×	✓
0.732	$SrRuO_3$	$Pnma$ (62)	$Pn'm'a$ (62.446)	$m'm'm$	×	✓
0.733	$AgRuO_3$	$R\bar{3}c$ (167)	$R\bar{3}'c'$ (167.106)	$\bar{3}'m'$	PT-wP	×
0.734	$Mn_3Ta_2O_8$	$I4_1/a$ (88)	$C2'/c$ (15.87)	$2'/m$	PT-wP	×
0.735	$LaBaMn_2O_5$	$P4/nmm$ (129)	$P4/nm'm'$ (129.417)	$4/mm'm'$	×	✓
0.736	$LaBaMn_2O_6$	$Pm\bar{3}m$ (221)	$P4/mm'm'$ (123.345)	$4/mm'm'$	×	✓
0.737	$LaBaMn_2O_6$	$P4/mmm$ (123)	$P4/mm'm'$ (123.345)	$4/mm'm'$	×	✓
0.738	$LaBaMn_2O_6$	$P4/mmm$ (123)	$P4/mm'm'$ (123.345)	$4/mm'm'$	×	✓
0.739	$YBaMn_2O_5$	$P4/nmm$ (129)	$P4/nm'm'$ (129.417)	$4/mm'm'$	×	✓
0.740	$Dy_3Ga_5O_{12}$	$Ia\bar{3}d$ (230)	$Ia\bar{3}d'$ (230.148)	$m\bar{3}m'$	×	×
0.741	$Er_3Ga_5O_{12}$	$Ia\bar{3}d$ (230)	$Ia\bar{3}d'$ (230.148)	$m\bar{3}m'$	×	×
0.742	$Tb_3Ga_5O_{12}$	$Ia\bar{3}d$ (230)	$Ia\bar{3}d'$ (230.148)	$m\bar{3}m'$	×	×
0.743	$Ho_3Al_5O_{12}$	$Ia\bar{3}d$ (230)	$Ia\bar{3}d'$ (230.148)	$m\bar{3}m'$	×	×
0.744	$Tb_3Al_5O_{12}$	$Ia\bar{3}d$ (230)	$Ia\bar{3}d'$ (230.148)	$m\bar{3}m'$	×	×
0.745	$Ho_3Ga_5O_{12}$	$Ia\bar{3}d$ (230)	$Ia\bar{3}d'$ (230.148)	$m\bar{3}m'$	×	×
0.746	$Tb_3Ga_5O_{12}$	$Ia\bar{3}d$ (230)	$Ia\bar{3}d'$ (230.148)	$m\bar{3}m'$	×	×
0.747	$Ba_3CoIr_2O_9$	$C2/c$ (15)	$C2/c$ (15.85)	$2/m$	×	✓
0.748	$Ba_3NiRu_2O_9$	$P6_3/mmc$ (194)	$P6_3'/m'm'c$ (194.268)	$6'/m'mm'$	×	×
0.749	$Ba_3CoRu_2O_9$	$Cmcm$ (63)	P_Bnma (62.454)	$mmm1'$	×	×
0.750	$Ba_3CoRu_2O_9$	$P6_3/mmc$ (194)	P_Bnma (62.454)	$mmm1'$	×	×
0.751	$Ca_2YZr_2Fe_3O_{12}$	$Ia\bar{3}d$ (230)	$R\bar{3}'c$ (167.105)	$\bar{3}'m$	PT-wP	×
0.752	$Ca_2YZr_2Fe_3O_{12}$	$Ia\bar{3}d$ (230)	$R\bar{3}'c$ (167.105)	$\bar{3}'m$	PT-wP	×
0.753	$Ca_2LaZr_2Fe_3O_{12}$	$Ia\bar{3}d$ (230)	$R\bar{3}'c$ (167.105)	$\bar{3}'m$	PT-wP	×
0.754	$Ca_2LaZr_2Fe_3O_{12}$	$Ia\bar{3}d$ (230)	$R\bar{3}'c$ (167.105)	$\bar{3}'m$	PT-wP	×
0.755	$Mn_2SeO_3F_2$	$Pnma$ (62)	$Pn'ma'$ (62.448)	$m'm'm$	×	✓
0.756	GaV_4S_8	$R3m$ (160)	$R3m'$ (160.67)	$3m'$	BW-woP	✓
0.757	$CeFeO_3$	$Pbnm$ (62)	$Pn'ma'$ (62.448)	$m'm'm$	×	✓
0.758	$CeFeO_3$	$Pbnm$ (62)	$Pnma$ (62.441)	mmm	×	×
0.759	$CeFeO_3$	$Pbnm$ (62)	$Pnma$ (62.441)	mmm	×	×
0.760	$FeOHSO_4$	$C2/c$ (15)	$C2'/c'$ (15.89)	$2'/m'$	×	✓
0.761	$SrFe_2Se_2O$	$Pmmn$ (59)	$Pm'm'n'$ (59.411)	$m'm'm'$	PT-wP	×
0.762	$SrFe_2S_2O$	$Pmmn$ (59)	$Pm'm'n'$ (59.411)	$m'm'm'$	PT-wP	×
0.763	$Mn_5(PO_4)_2(PO_3(OH))_2(H_2O)_4$	$C2/c$ (15)	$C2'/c'$ (15.89)	$2'/m'$	×	✓
0.764	$Mn_5(PO_4)_2(PO_3(OH))_2(H_2O)_4$	$C2/c$ (15)	$C2'/c'$ (15.89)	$2'/m'$	×	✓
0.765	$Mn_5(PO_4)_2(PO_3(OH))_2(H_2O)_4$	$C2/c$ (15)	$C2'/c'$ (15.89)	$2'/m'$	×	✓
0.766	$YbMnSb_2$	$P4/nmm$ (129)	$P4'/n'm'm$ (129.416)	$4'/m'm'm$	PT-wP	×
0.767	$SrMnSb_2$	$Pnma$ (62)	$Pn'ma'$ (62.448)	$m'm'm$	×	✓
0.768	$SrMnSb_2$	$Pnma$ (62)	$Pn'a'2_1$ (33.148)	$m'm'2$	BW-wP	✓
0.769	$YbMnBi_2$	$P4/nmm$ (129)	$P4'/n'm'm$ (129.416)	$4'/m'm'm$	PT-wP	×
0.770	$Fe_2Co_2Nb_2O_9$	$P\bar{3}1c$ (165)	$C2/c'$ (15.88)	$2/m'$	PT-wP	×
0.771	$PrMnSi_2$	$Cmcm$ (63)	$Cm'cm'$ (63.464)	$m'm'm$	×	✓
0.772	$PrMnSi_2$	$Cmcm$ (63)	$Cm'cm'$ (63.464)	$m'm'm$	×	✓
0.773	$NdMnSi_2$	$Cmcm$ (63)	$C2'/m'$ (12.62)	$2'/m'$	×	✓

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BCS-ID	Formula	Parent	MSG	MPG	SHG type	LMO
0.774	$NdMnSi_2$	$Cmcm$ (63)	$Cm'cm'$ (63.464)	$m'm'm$	×	✓
0.775	$NdMnSi_2$	$Cmcm$ (63)	$Cm'cm'$ (63.464)	$m'm'm$	×	✓
0.776	$CeMnSi_2$	$Cmcm$ (63)	$Cm'cm'$ (63.464)	$m'm'm$	×	✓
0.777	$CeMnSi_2$	$Cmcm$ (63)	$Cm'cm'$ (63.464)	$m'm'm$	×	✓
0.778	$LaMnSi_2$	$Cmcm$ (63)	$Cm'cm'$ (63.464)	$m'm'm$	×	✓
0.779	$LaMnSi_2$	$Cmcm$ (63)	$Cm'cm'$ (63.464)	$m'm'm$	×	✓
0.780	$LaMnSi_2$	$Cmcm$ (63)	$Cm'cm'$ (63.464)	$m'm'm$	×	✓
0.781	$CeMnSi_2$	$Cmcm$ (63)	$Cm'cm'$ (63.464)	$m'm'm$	×	✓
0.782	$NdScO_3$	$Pbnm$ (62)	$Pnm'a$ (62.444)	$m'mm$	PT-wP	×
0.783	$NdInO_3$	$Pbnm$ (62)	$Pnm'a$ (62.444)	$m'mm$	PT-wP	×
0.784	$NdCoO_3$	$Pbnm$ (62)	$Pnma$ (62.441)	mmm	×	×
0.785	$NdVO_3$	$Pbnm$ (62)	$P2_1'/m'$ (11.54)	$2'/m'$	×	✓
0.786	$NdVO_3$	$Pbnm$ (62)	$P2_1'/m'$ (11.54)	$2'/m'$	×	✓
0.787	YVO_3	$Pbnm$ (62)	$Pn'm'a$ (62.446)	$m'm'm$	×	✓
0.788	YVO_3	$P2_1/b11$ (14)	$P\bar{1}$ (2.4)	$\bar{1}$	×	✓
0.789	$CeCuSi$	$P6_3/mmc$ (194)	$Cmc'm'$ (63.463)	$m'm'm$	×	✓
0.790	Sr_2DyRuO_6	$P2_1/n$ (14)	$P2_1'/c'$ (14.79)	$2'/m'$	×	✓
0.791	Sr_2TbRuO_6	$P2_1/n$ (14)	$P2_1/c$ (14.75)	$2/m$	×	✓
0.792	Sr_2HoRuO_6	$P2_1/n$ (14)	$P2_1/c$ (14.75)	$2/m$	×	✓
0.793	Sr_2HoRuO_6	$P2_1/n$ (14)	$P2_1/c$ (14.75)	$2/m$	×	✓
0.794	Sr_2HoRuO_6	$P2_1/n$ (14)	$P2_1/c$ (14.75)	$2/m$	×	✓
0.795	Sr_2YRuO_6	$P2_1/c$ (14)	$P2_1/c$ (14.75)	$2/m$	×	✓
0.796	Ca_2NiOsO_6	$P2_1/n$ (14)	$P2_1'/c'$ (14.79)	$2'/m'$	×	✓
0.797	$SmBaMn_2O_5$	$P4/nmm$ (129)	$P4/nm'm'$ (129.417)	$4/mm'm'$	×	✓
0.798	$MnPd_2$	$Pnma$ (62)	$Pnma'$ (62.445)	$m'mm$	PT-wP	×
0.799	$Sr_2Co_2O_5$	$Ima2$ (46)	P_Inc2 (30.122)	$mm2_1'$	G-woP	×
0.800	$MnTe$	$P6_3/mmc$ (194)	$Cmcm$ (63.457)	mmm	×	×
0.801	$Tl_3Fe_2S_4$	$Pnma$ (62)	$Pnma'$ (62.445)	$m'mm$	PT-wP	×
0.802	$CuFeS_2$	$I\bar{4}2d$ (122)	$I\bar{4}2d$ (122.333)	$\bar{4}2m$	O-woP	×
0.803	$NbMnP$	$Pnma$ (62)	$Pm'n2_1'$ (31.125)	$m'm2'$	BW-wP	✓
0.804	MoP_3SiO_{11}	$R\bar{3}c$ (167)	$C2/c'$ (15.88)	$2/m'$	PT-wP	×
0.805	$DyBaCuO_5$	$Pnma$ (62)	$Pnm'a$ (62.444)	$mm'm$	PT-wP	×
0.806	$Fe_2Se_2O_7$	$Pccn$ (56)	$Pc'cn$ (56.367)	$m'mm$	PT-wP	×
0.807	$Fe_2Se_2O_7$	$Pccn$ (56)	$Pc'cn$ (56.367)	$m'mm$	PT-wP	×
0.808	$Fe_2Se_2O_7$	$Pccn$ (56)	$Pc'cn$ (56.367)	$m'mm$	PT-wP	×
0.809	Fe_2WO_6	$P2_1/c$ (14)	$P2_1/c'$ (14.78)	$2/m'$	PT-wP	×
0.810	Fe_2WO_6	$Pbcn$ (60)	$Pbc'n'$ (60.423)	$m'm'm$	×	✓
0.811	Fe_2WO_6	$Pbcn$ (60)	$Pbc'n'$ (60.423)	$m'm'm$	×	✓
0.812	Fe_2WO_6	$Pbcn$ (60)	$Pn'c2'$ (30.113)	$m'm2'$	BW-wP	✓
0.813	Fe_2WO_6	$Pbcn$ (60)	$Pbc'n'$ (60.423)	$m'm'm$	×	✓
0.814	Fe_2WO_6	$Pbcn$ (60)	$Pb'cn$ (60.419)	$m'mm$	PT-wP	×
0.815	$MnNb_2O_6$	$Pbcn$ (60)	$Pb'cn$ (60.419)	$m'mm$	PT-wP	×
0.816	$MnTa_2O_6$	$Pbcn$ (60)	$Pb'cn$ (60.419)	$m'mm$	PT-wP	×
0.817	$Mn(Nb_{0.5}Ta_{0.5})_2O_6$	$Pbcn$ (60)	$Pb'cn$ (60.419)	$m'mm$	PT-wP	×
0.818	$MnTa_2O_6$	$Pbcn$ (60)	$Pb'cn$ (60.419)	$m'mm$	PT-wP	×
0.819	$MnNb_2O_6$	$Pbcn$ (60)	$Pb'cn$ (60.419)	$m'mm$	PT-wP	×
0.820	$Bi_{0.85}Ca_{0.15}Fe_{0.55}Mn_{0.45}O_3$	$Pnma$ (62)	$Pn'm'a$ (62.446)	$m'm'm$	×	✓
0.821	$SrGd_2O_4$	$Pnma$ (62)	$Pnma'$ (62.445)	$m'mm$	PT-wP	×
0.822	Nd_2ScNbO_7	$Fd\bar{3}m$ (227)	$Fd\bar{3}m'$ (227.131)	$m\bar{3}m'$	×	×
0.823	Sr_2MnGaO_5	$Ima2$ (46)	$Im'a2'$ (46.243)	$m'm2'$	BW-woP	✓
0.824	$Sr_2MnGaO_{5.5}$	$P4/mmm$ (123)	P_C4/mbm (127.397)	$4/mmm1'$	×	×
0.825	Ca_2MnGaO_5	$Pnma$ (62)	$Pnm'a'$ (62.447)	$m'm'm$	×	✓
0.826	$MnTeLi0.00_3$	$P6_3/mmc$ (194)	$C2'/m'$ (12.62)	$2'/m'$	×	✓
0.827	Na_2MnPO_4F	$P2_1/c$ (14)	$P2_1/c'$ (14.78)	$2/m'$	PT-wP	×
0.828	Na_2MnPO_4F	$P2_1/n$ (14)	$P2_1/c'$ (14.78)	$2/m'$	PT-wP	×
0.829	Na_2MnPO_4F	$P2_1/n$ (14)	$P2_1/c'$ (14.78)	$2/m'$	PT-wP	×
0.830	Na_2MnPO_4F	$P2_1/n$ (14)	$P2_1/c'$ (14.78)	$2/m'$	PT-wP	×
0.831	$BaCaFe_4O_7$	$Pbn2_1$ (33)	$Pn'a'2_1$ (33.148)	$m'm'2$	BW-woP	✓

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BCS-ID	Formula	Parent	MSG	MPG	SHG type	LMO
0.832	$CeAuGe$	$P6_3mc$ (186)	$Cmc'2_1'$ (36.175)	$m'm2'$	BW-woP	✓
0.833	$CeCuGe$	$P6_3/mmc$ (194)	$Cmc'm'$ (63.463)	$m'm'm$	×	✓
0.834	$CrSbSe_3$	$Pnma$ (62)	$Pnm'a'$ (62.447)	$m'm'm$	×	✓
0.835	$Dy_5Pd_2In_4$	$PPbam$ (55)	$Pb'a'm$ (55.357)	$m'm'm$	×	✓
1.0.1	Ag_2CrO_2	$P\bar{3}m1$ (164)	$C2'/m$ (12.60)	$2'/m$	PT-wP	×
1.0.2	$URu_{0.96}Rh_{0.04}Si_2$	$I4/mmm$ (139)	$Im'm'm$ (71.536)	$m'm'm$	×	✓
1.0.3	$CsCoBr_3$	$P6_3/mmc$ (194)	$Cm'c2_1'$ (36.174)	$m'm2'$	BW-wP	✓
1.0.4	$CsNiCl_3$	$P6_3/mmc$ (194)	$C22'2_1'$ (20.34)	$2'2'2$	BW-wP	✓
1.0.5	Sr_3CoIrO_6	$R\bar{3}c$ (167)	$P\bar{3}c'1$ (165.95)	$\bar{3}m'$	×	✓
1.0.6	CoV_2O_6	$C2/m$ (12)	$C2'/m'$ (12.62)	$2'/m'$	×	✓
1.0.7	$LuFe_2O_4$	$R\bar{3}m$ (166)	$C2'/m'$ (12.62)	$2'/m'$	×	✓
1.0.8	$Ba_3MnNb_2O_9$	$P\bar{3}m1$ (164)	$P31m$ (157.53)	$3m$	O-wP	×
1.0.9	$CsCoCl_3$	$P6_3/mmc$ (194)	$P6_3'/m'cm'$ (193.259)	$6'/m'mm'$	×	×
1.0.10	Sr_3NiIrO_6	$R\bar{3}c$ (167)	$P\bar{3}c'1$ (165.95)	$\bar{3}m'$	×	✓
1.0.11	$CeCoGe_3$	$I4mm$ (107)	$I4m'm'$ (107.231)	$4m'm'$	BW-woP	✓
1.0.12	UAu_2Si_2	$I4/mmm$ (139)	$Im'm'm$ (71.536)	$m'm'm$	×	✓
1.0.13	FeI_2	$P\bar{3}m1$ (164)	$C2'/m'$ (12.62)	$2'/m'$	×	✓
1.0.14	$CsFeCl_3$	$P6_3/mmc$ (194)	$P\bar{6}'2'm$ (189.223)	$\bar{6}'m2'$	BW-wP	×
1.0.15	$La_{0.33}Sr_{0.67}FeO_3$	$R\bar{3}c$ (167)	$P322_1$ (154.41)	32	O-wP	×
1.0.16	$La_{0.33}Sr_{0.67}FeO_3$	$R\bar{3}c$ (167)	$C2/c$ (15.85)	$2/m$	×	✓
1.0.17	$CaBaCo_2Fe_2O_7$	$P6_3mc$ (186)	$P31m'$ (157.55)	$3m'$	BW-woP	✓
1.0.18	$Cs_2MnU_3F_{16}$	$P6_3/mmc$ (194)	$P6_3/mc'm'$ (193.260)	$6/mm'm'$	×	✓
1.0.19	$Cs_2CoU_3F_{16}$	$P6_3/mmc$ (194)	$P6_3/mc'm'$ (193.260)	$6/mm'm'$	×	✓
1.0.20	$Cs_2NiU_3F_{16}$	$P6_3/mmc$ (194)	$P6_3/mc'm'$ (193.260)	$6/mm'm'$	×	✓
1.0.21	$K_2Mn_3(VO_4)_2CO_3$	$P6_3/m$ (176)	$P6_3'/m$ (176.145)	$6'/m$	PT-wP	×
1.0.22	$K_2Mn_3(VO_4)_2CO_3$	$P6_3/m$ (176)	$P2_1'$ (4.9)	$2'$	BW-wP	✓
1.0.23	$Dy_3Ru_4Al_{12}$	$P6_3/mmc$ (194)	$C2'/m'$ (12.62)	$2'/m'$	×	✓
1.0.24	$ThMn_2$	$P6_3/mmc$ (194)	$P\bar{6}'2'm$ (189.223)	$\bar{6}'m2'$	BW-wP	×
1.0.25	$CaBaCo_3FeO_7$	$Pna2_1$ (33)	$Pn'a'2_1$ (33.148)	$m'm'2$	BW-woP	✓
1.0.26	$RbCoBr_3$	$P6_3/mmc$ (194)	$P6_3'/m'cm'$ (193.259)	$6'/m'mm'$	×	×
1.0.27	Li_2MnTeO_6	$P\bar{3}1c$ (163)	$P\bar{3}c1$ (165.91)	$\bar{3}m$	×	×
1.0.28	$Tb(DCO_2)_3$	$R3m$ (160)	$P3m'1$ (156.51)	$3m'$	BW-woP	✓
1.0.29	$CeIrGe_3$	$I4mm$ (107)	$I4m'm'$ (107.231)	$4m'm'$	BW-woP	✓
1.0.30	$LaCa_2Fe_3O_9$	$Pnma$ (62)	$Pmn2_1$ (31.123)	$mm2$	O-wP	×
1.0.31	$EuIn_2As_2$	$P6_3/mmc$ (194)	$C2'2'2_1$ (20.33)	$2'2'2$	BW-wP	✓
1.0.32	$EuIn_2As_2$	$P6_3/mmc$ (194)	$P612'2'$ (178.159)	$62'2'$	BW-wP	✓
1.0.33	FeF_3	$P6/mmm$ (191)	$P6_3/m$ (176.143)	$6/m$	×	✓
1.0.34	$RbNiCl_3$	$P6_3/mmc$ (194)	$Cm'c2_1'$ (36.174)	$m'm2'$	BW-wP	✓
1.0.35	$CsMnBr_3$	$P6_3/mmc$ (194)	$P\bar{6}2'm'$ (189.225)	$\bar{6}m'2'$	BW-wP	✓
1.0.36	$CsMnI_3$	$P6_3/mmc$ (194)	$Cm'c2_1'$ (36.174)	$m'm2'$	BW-wP	✓
1.0.37	$CsMnI_3$	$P6_3/mmc$ (194)	$Cm'c2_1'$ (36.174)	$m'm2'$	BW-wP	✓
1.0.38	$CsCoCl_3$	$P6_3/mmc$ (194)	$P6_3'/m'cm'$ (193.259)	$6'/m'mm'$	×	×
1.0.39	$BaMnO_3$	$P6_3/mmc$ (194)	$P6_3'/m'cm'$ (193.259)	$6'/m'mm'$	×	×
1.0.40	$RbFeCl_3$	$P6_3/mmc$ (194)	$P\bar{6}'2m'$ (189.224)	$\bar{6}'m'2$	BW-wP	×
1.0.41	$RbNiCl_3$	$P6_3/mmc$ (194)	$C22'2_1'$ (20.34)	$2'2'2$	BW-wP	✓
1.0.42	$CsNiCl_3$	$P6_3/mmc$ (194)	$C22'2_1'$ (20.34)	$2'2'2$	BW-wP	✓
1.0.43	UPd_2Si_2	$I4/mmm$ (139)	$I4/mm'm'$ (139.537)	$4/mm'm'$	×	✓
1.0.44	$Ba_3CoSb_2O_9$	$P6_3/mmc$ (194)	$Cm'c2_1'$ (36.174)	$m'm2'$	BW-wP	✓
1.0.45	$Ba_3CoSb_2O_9$	$P6_3/mmc$ (194)	$P\bar{6}2m$ (189.221)	$\bar{6}m2$	O-wP	×
1.0.46	$Ba_3MnSb_2O_9$	$C2/c$ (15)	$C2$ (5.13)	2	O-wP	✓
1.0.47	$MnSe_2$	$Pa\bar{3}$ (205)	$Pbca$ (61.433)	mmm	×	×

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BCS-ID	Formula	Parent	MSG	MPG	SHG type	LMO
1.0.48	$MnSe_2$	$Pa\bar{3}$ (205)	$Pca'2_1'$ (29.102)	$m'm2'$	BW-wP	✓
1.0.49	$BaCoSiO_4$	$P6_3$ (173)	$P6_3$ (173.129)	6	O-woP	✓
1.0.50	$CoGeO_3$	$C2/c$ (15)	$C2'/c'$ (15.89)	$2'/m'$	×	✓
1.0.51	Na_2MnTeO_6	$P\bar{3}1c$ (163)	$R\bar{3}'c'$ (167.106)	$\bar{3}'m'$	PT-wP	×
1.0.52	$Tb_{14}Ag_{51}$	$P6/m$ (175)	$P\bar{6}'$ (174.135)	$\bar{6}'$	BW-wP	×
1.1	Mn_3O_4	$Pbcm$ (57)	P_cnma (62.452)	$mmm1'$	×	×
1.2	$CuSe_2O_5$	$C2/c$ (15)	P_c2_1/c (14.84)	$2/m1'$	×	×
1.3	Sr_2IrO_4	$I4_1/acd$ (142)	P_Icca (54.352)	$mmm1'$	×	×
1.4	$YBa_2Cu_3O_{6+d}$	$P4/mmm$ (123)	C_ammm (65.489)	$mmm1'$	×	×
1.5	$YBa_2Cu_3O_{6+d}$	$P4/mmm$ (123)	F_Smmm (69.526)	$mmm1'$	×	×
1.6	NiO	$Fm\bar{3}m$ (225)	C_c2/c (15.90)	$2/m1'$	×	×
1.7	$NdFe_3B_4O_{12}$	$R32$ (155)	C_c2 (5.16)	$21'$	G-woP	×
1.8	$CeRu_2Al_{10}$	$Cmcm$ (63)	P_Cbcm (57.391)	$mmm1'$	×	×
1.9	Li_2VOSiO_4	$P4/nmm$ (129)	P_Abcm (57.389)	$mmm1'$	×	×
1.1	Na_2IrO_3	$C2/m$ (12)	C_c2/m (12.63)	$2/m1'$	×	×
1.11	$Bi_4Fe_5O_{13}F$	$P4_2/mbc$ (135)	P_C42/n (86.73)	$4/m1'$	×	×
1.12	$BaNd_{0.9}Y_{0.1}MoO_6$	$I4/m$ (87)	P_I4/m (83.50)	$4/m1'$	×	×
1.13	$Ba_3Nb_2NiO_9$	$P\bar{3}m1$ (164)	P_c31c (159.64)	$3m1'$	G-wP	×
1.14	Ho_2BaNiO_5	$Immm$ (71)	C_c2/c (15.90)	$2/m1'$	×	×
1.15	Er_2BaNiO_5	$Immm$ (71)	C_c2/c (15.90)	$2/m1'$	×	×
1.16	$BaFe_2As_2$	$I4/mmm$ (139)	C_Amca (64.480)	$mmm1'$	×	×
1.17	CoV_2O_6-alpha	$C2/m$ (12)	C_c2/c (15.90)	$2/m1'$	×	×
1.18	MnS_2	$Pa\bar{3}$ (205)	P_bca2_1 (29.105)	$mm21'$	G-wP	×
1.19	$PrMn_2O_5$	$Pbam$ (55)	P_aca2_1 (29.104)	$mm21'$	G-wP	×
1.20	$HoMnO_3$	$Pnma$ (62)	P_bmn2_1 (31.129)	$mm21'$	G-wP	×
1.21	$DyCo_2Si_2$	$I4/mmm$ (139)	P_I4/mnc (128.410)	$4/mmm1'$	×	×
1.22	$DyCu_2Si_2$	$I4/mmm$ (139)	C_c2/m (12.63)	$2/m1'$	×	×
1.23	La_2CuO_4	$Cmce$ (64)	P_Accn (56.374)	$mmm1'$	×	×
1.24	ZnV_2O_4	$I4_1/amd$ (141)	P_I432_12 (96.150)	$4221'$	G-wP	×
1.25	$KFe_3(OH)_6(SO_4)_2$	$R\bar{3}m$ (166)	$R_I\bar{3}c$ (167.108)	$\bar{3}m1'$	×	×
1.26	$CsFe_2Se_3$	$Cmcm$ (63)	P_c2_1/c (14.82)	$2/m1'$	×	×
1.27	$TaFe_{1+y}Te_3$	$P2_1/m$ (11)	P_c2_1/c (14.82)	$2/m1'$	×	×
1.28	CrN	$Fm\bar{3}m$ (225)	P_anma (62.450)	$mmm1'$	×	×
1.29	$LaSrFeO_4$	$I4/mmm$ (139)	C_Amca (64.480)	$mmm1'$	×	×
1.30	$BaCo_2V_2O_8$	$I4_1/acd$ (142)	P_Icca (54.352)	$mmm1'$	×	×
1.31	MnO	$Fm\bar{3}m$ (225)	C_c2/c (15.90)	$2/m1'$	×	×
1.32	Lu_2MnCoO_6	$P2_1/n$ (14)	P_a2_1 (4.10)	$21'$	G-wP	×
1.33	$ErAuGe$	$P6_3mc$ (186)	P_Cna2_1 (33.154)	$mm21'$	G-woP	×
1.34	$HoAuGe$	$P6_3mc$ (186)	P_Cna2_1 (33.154)	$mm21'$	G-woP	×
1.35	$LiErF_4$	$I4_1/a$ (88)	P_C2_1/c (14.84)	$2/m1'$	×	×
1.36	Dy_2BaNiO_5	$Immm$ (71)	C_c2/c (15.90)	$2/m1'$	×	×
1.37	$VOCl$	$Pmmn$ (59)	C_a2/c (15.91)	$2/m1'$	×	×
1.38	Nd_2NaOsO_6	$P2_1/n$ (14)	$P_S\bar{1}$ (2.7)	$\bar{1}1'$	×	×
1.39	$LiFeGe_2O_6$	$P2_1/c$ (14)	P_a2_1/c (14.80)	$2/m1'$	×	×
1.40	$SrNdFeO_4$	$I4/mmm$ (139)	C_Accm (66.5)	$mmm1'$	×	×
1.41	$SrNdFeO_4$	$I4/mmm$ (139)	C_Amca (64.480)	$mmm1'$	×	×
1.42	La_2NiO_4	$Bmeb$ (64)	P_Cmna (53.335)	$mmm1'$	×	×
1.43	$PrNiO_3$	$Pbnm$ (62)	C_amc2_1 (36.178)	$mm21'$	G-wP	×
1.44	$NdNiO_3$	$Pbnm$ (62)	C_amc2_1 (36.178)	$mm21'$	G-wP	×
1.45	$NdNiO_3$	$Pbnm$ (62)	C_amc2_1 (36.178)	$mm21'$	G-wP	×
1.46	Sr_2FeOsO_6	$I4/m$ (87)	P_c4/n (85.64)	$4/m1'$	×	×
1.47	Sr_2FeOsO_6	$I4/m$ (87)	P_I4/m (83.50)	$4/m1'$	×	×
1.48	$HoNiO_3$	$P2_1/n$ (14)	P_a2_1 (4.10)	$21'$	G-wP	×
1.49	Ag_2NiO_2	$C2/m$ (12)	C_c2/c (15.90)	$2/m1'$	×	×
1.50	$AgNiO_2$	$P6_322$ (182)	$P_B2_12_12$ (18.22)	$2221'$	G-woP	×
1.51	Cs_2CoCl_4	$Pnma$ (62)	P_a2_1 (4.10)	$21'$	G-wP	×
1.52	$CaFe_2As_2$	$I4/mmm$ (139)	C_Amca (64.480)	$mmm1'$	×	×

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TABLE S1 – continued from previous page

BCS-ID	Formula	Parent	MSG	MPG	SHG type	LMO
1.53	Er_2BaNiO_5	$Immm$ (71)	C_c2/c (15.90)	$2/m1'$	×	×
1.54	$GdMn_2O_5$	$Pbam$ (55)	P_aca2_1 (29.104)	$mm21'$	G-wP	×
1.55	Na_2MnF_5	$P2_1/c$ (14)	P_bc (7.29)	$m1'$	G-wP	×
1.56	$Gd_2Ti_2O_7$	$Fd\bar{3}m$ (227)	$R_I\bar{3}m$ (166.102)	$\bar{3}m1'$	×	×
1.57	$CuMnO_2$	$C2/m$ (12)	$P_S\bar{1}$ (2.7)	$\bar{1}1'$	×	×
1.58	$La_2O_2Fe_2OSe_2$	$I4/mmm$ (139)	C_cc (9.40)	$m1'$	G-wP	×
1.59	KTb_3F_{12}	$I4/m$ (87)	P_I42/m (84.58)	$4/m1'$	×	×
1.60	$Ca_3Co_2O_6$	$R\bar{3}c$ (167)	P_C2_1/c (14.84)	$2/m1'$	×	×
1.61	$MnWO_4$	$P2/c$ (13)	C_a2/c (15.91)	$2/m1'$	×	×
1.62	CuO	$C2/c$ (15)	P_a2_1/c (14.80)	$2/m1'$	×	×
1.63	$MnPb_4Sb_6S_{14}$	$P2_1/c$ (14)	P_a2_1/c (14.80)	$2/m1'$	×	×
1.64	$BaNiF_4$	$Cmc2_1$ (36)	P_a2_1 (4.10)	$21'$	G-woP	×
1.65	$SrFeO_2$	$P4/mmm$ (123)	F_Smmm (69.526)	$mmm1'$	×	×
1.66	$Fe(ND_3)_2PO_4$	$P2_1/n$ (14)	$P_S\bar{1}$ (2.7)	$\bar{1}1'$	×	×
1.67	$TmPtIn$	$P\bar{6}2m$ (189)	A_bbm2 (39.201)	$mm21'$	G-woP	×
1.68	$NaNdFeWO_6$	$P2_1$ (4)	P_S1 (1.3)	$11'$	G-woP	×
1.69	CoO	$Fm\bar{3}m$ (225)	C_c2/c (15.90)	$2/m1'$	×	×
1.70	CoV_2O_6	$C2/m$ (12)	C_c2/c (15.90)	$2/m1'$	×	×
1.71	$SrCo_2V_2O_8$	$I4_1cd$ (110)	P_Ica2_1 (29.110)	$mm21'$	G-woP	×
1.72	Sr_2CoOsO_6	$I4/m$ (87)	C_c2/c (15.90)	$2/m1'$	×	×
1.73	CaV_2O_4	$P2_1/n11$ (14)	P_a2_1/c (14.80)	$2/m1'$	×	×
1.74	$BiMn_2O_5$	$Pbam$ (55)	C_amc2_1 (36.178)	$mm21'$	G-wP	×
1.75	$BiMn_2O_5$	$Pbam$ (55)	C_am (8.36)	$m1'$	G-wP	×
1.76	$DyMn_2O_5$	$Pbam$ (55)	P_aca2_1 (29.104)	$mm21'$	G-wP	×
1.77	Sr_2IrO_4	$I4_1/acd$ (142)	P_Icca (54.352)	$mmm1'$	×	×
1.78	Li_2MnSiO_4	$P2_1/n$ (14)	P_a2_1/c (14.80)	$2/m1'$	×	×
1.79	Li_2CoSiO_4	$Pna2_1$ (33)	C_ac (9.41)	$m1'$	G-woP	×
1.80	Dy_2CoGa_8	$P4/mmm$ (123)	I_c4/mcm (140.550)	$4/mmm1'$	×	×
1.81	$GdIn_3$	$Pm\bar{3}m$ (221)	P_C4/mbm (127.397)	$4/mmm1'$	×	×
1.82	Nd_2RhIn_8	$P4/mmm$ (123)	I_c4/mcm (140.550)	$4/mmm1'$	×	×
1.83	$BaFeO_{2.5}$	$P2_1/c$ (14)	P_a2_1/c (14.80)	$2/m1'$	×	×
1.84	$SrFeO_2F$	$Pm\bar{3}m$ (221)	I_c4/mcm (140.550)	$4/mmm1'$	×	×
1.85	alpha-Mn	$I\bar{4}3m$ (217)	$P_I\bar{4}2_1c$ (114.282)	$\bar{4}2m1'$	G-woP	×
1.86	GeV_4S_8	$F\bar{4}3m$ (216)	P_ana2_1 (33.149)	$mm21'$	G-woP	×
1.87	Tb_2CoGa_8	$P4/mmm$ (123)	I_c4/mcm (140.550)	$4/mmm1'$	×	×
1.88	Mn_5Si_3	$P6_3/mcm$ (193)	P_Cbcn (60.431)	$mmm1'$	×	×
1.89	$DyFe_3(BO_3)_4$	$P312_1$ (152)	P_c322_1 (154.44)	$321'$	G-woP	×
1.90	$YFe_3(BO_3)_4$	$P312_1$ (152)	C_c2 (5.16)	$21'$	G-woP	×
1.91	$TbFe_3(BO_3)_4$	$P312_1$ (152)	P_c322_1 (154.44)	$321'$	G-woP	×
1.92	$HoFe_3(BO_3)_4$	$P312_1$ (152)	P_c322_1 (154.44)	$321'$	G-woP	×
1.93	$HoFe_3(BO_3)_4$	$P312_1$ (152)	P_S1 (1.3)	$11'$	G-woP	×
1.94	$Ba_3LaRu_2O_9$	$P6_3/mmc$ (194)	P_C2_1/c (14.84)	$2/m1'$	×	×
1.95	$BaNd_2O_4$	$Pnam$ (62)	P_a2_1/c (14.80)	$2/m1'$	×	×
1.96	$BaNd_2O_4$	$Pnam$ (62)	P_a2_1/c (14.80)	$2/m1'$	×	×
1.97	Li_2MnO_3	$C2/m$ (12)	C_c2/m (12.63)	$2/m1'$	×	×
1.98	$DyFe_4Ge_2$	$P4_2/mnm$ (136)	P_cc2 (27.82)	$mm21'$	G-wP	×
1.99	$CsCoCl_3(D_2O)_2$	$Pcca$ (54)	P_bccn (56.372)	$mmm1'$	×	×
1.100	Cu_2MnSnS_4	$I\bar{4}2m$ (121)	C_c2 (5.16)	$21'$	G-woP	×
1.101	$LuMnO_3$	$Pbnm$ (62)	P_bmn2_1 (31.129)	$mm21'$	G-wP	×
1.102	U_2Ni_2In	$P4/mbm$ (127)	P_c4/mnc (128.408)	$4/mmm1'$	×	×
1.103	U_2Rh_2Sn	$P4/mbm$ (127)	P_c4_2/mbc (135.492)	$4/mmm1'$	×	×
1.104	Gd_2CuO_4	$I4/mmm$ (139)	C_Accm (66.5)	$mmm1'$	×	×
1.105	Gd_2CuO_4	$Aeam$ (64)	P_Accn (56.374)	$mmm1'$	×	×
1.106	Pr_2CuO_4	$I4/mmm$ (139)	C_Accm (66.5)	$mmm1'$	×	×
1.107	Sm_2CuO_4	$I4/mmm$ (139)	C_Amca (64.480)	$mmm1'$	×	×
1.108	$TbMn_2O_5$	$Pbam$ (55)	C_am (8.36)	$m1'$	G-wP	×
1.109	$HoMn_2O_5$	$Pbam$ (55)	C_am (8.36)	$m1'$	G-wP	×
1.110	$ScMn_6Ge_6$	$P6/mmm$ (191)	P_c6/mcc (192.252)	$6/mmm1'$	×	×

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TABLE S1 – continued from previous page

BCS-ID	Formula	Parent	MSG	MPG	SHG type	LMO
1.111	GdBiPt	$F\bar{4}3m$ (216)	C_cc (9.40)	$m1'$	G-woP	×
1.112	$NiTa_2O_6$	$P4_2/mnm$ (136)	P_c2_1/c (14.82)	$2/m1'$	×	×
1.113	$NiSb_2O_6$	$P4_2/mnm$ (136)	$P_S\bar{1}$ (2.7)	$\bar{1}1'$	×	×
1.114	Ca_4IrO_6	$R\bar{3}c$ (167)	P_C2/c (13.74)	$2/m1'$	×	×
1.115	$Dy_3Ru_4Al_{12}$	$P6_3/mmc$ (194)	C_c2/c (15.90)	$2/m1'$	×	×
1.116	$AgMnVO_4$	$Pnma$ (62)	P_a2_1/m (11.55)	$2/m1'$	×	×
1.117	$NaFePO_4$	$Pnma$ (62)	P_c2_1/c (14.82)	$2/m1'$	×	×
1.118	$GdPO_4$	$P2_1/n$ (14)	P_a2_1/c (14.80)	$2/m1'$	×	×
1.119	$LaMn_3V_4O_{12}$	$Im\bar{3}$ (204)	$R_I\bar{3}$ (148.20)	$\bar{3}1'$	×	×
1.120	$BaFe_2Se_3$	$Pnma$ (62)	C_ac (9.41)	$m1'$	G-wP	×
1.121	$NaFeSO_4F$	$C2/c$ (15)	P_C2/c (13.74)	$2/m1'$	×	×
1.122	$Cu_3Bi(SeO_3)_2O_2Br$	$Pmmn$ (59)	P_cccn (56.373)	$mmm1'$	×	×
1.123	$Cu_3Y(SeO_3)_2O_2Cl$	$Pmmn$ (59)	P_cccn (56.373)	$mmm1'$	×	×
1.124	$YBaFe_4O_7$	$P2_1$ (4)	P_a2_1 (4.10)	$21'$	G-woP	×
1.125	LaFeAsO	$Cmme$ (67)	I_cbca (73.553)	$mmm1'$	×	×
1.126	$NaCoSO_4F$	$C2/c$ (15)	P_C2/c (13.74)	$2/m1'$	×	×
1.127	$BiNiO(PO_4)$	$P2_1/n$ (14)	P_a2_1/c (14.80)	$2/m1'$	×	×
1.128	$BiCoO(PO_4)$	$P2_1/n$ (14)	P_a2_1/c (14.80)	$2/m1'$	×	×
1.129	$AgFe_3(SO_4)_2(OD)_6$	$R\bar{3}m$ (166)	$R_I\bar{3}c$ (167.108)	$\bar{3}m1'$	×	×
1.130	Cr_2As	$P4/nmm$ (129)	P_anma (62.450)	$mmm1'$	×	×
1.131	Fe_2As	$P4/nmm$ (129)	P_anma (62.450)	$mmm1'$	×	×
1.132	Mn_2As	$P4/nmm$ (129)	P_anma (62.450)	$mmm1'$	×	×
1.133	$CuSb_2O_6$	$P2_1/n$ (14)	P_a2_1/c (14.80)	$2/m1'$	×	×
1.134	$Co_2C10O_8H_2$	$C2/m$ (12)	P_C2_1/m (11.57)	$2/m1'$	×	×
1.135	$C_8H10Co_2O_{11}$	$P\bar{1}$ (2)	$P_S\bar{1}$ (2.7)	$\bar{1}1'$	×	×
1.136	$AgCrS_2$	$R3m$ (160)	C_cm (8.35)	$m1'$	G-woP	×
1.137	Sr_2CaIrO_6	$P2_1/n$ (14)	$P_S\bar{1}$ (2.7)	$\bar{1}1'$	×	×
1.138	MgV_2O_4	$I\bar{4}m2$ (119)	C_A222_1 (20.37)	$2221'$	G-woP	×
1.139	Ho_2RhIn_8	$P4/mmm$ (123)	P_ccmm (49.273)	$mmm1'$	×	×
1.140	PrMgPb	$I4/mmm$ (139)	P_A2/c (13.73)	$2/m1'$	×	×
1.141	NdMgPb	$I4/mmm$ (139)	P_A2/c (13.73)	$2/m1'$	×	×
1.142	CeMgPb	$I4/mmm$ (139)	C_Ammma (67.510)	$mmm1'$	×	×
1.143	Mn_3Pt	$Pm\bar{3}m$ (221)	P_c4_2/mcm (132.456)	$4/mmm1'$	×	×
1.144	$NH_4FeCl_2(HCOO)$	$C2/c$ (15)	P_C2_1/c (14.84)	$2/m1'$	×	×
1.145	$Mn_3Ni_20P_6$	$Fm\bar{3}m$ (225)	C_Amca (64.480)	$mmm1'$	×	×
1.146	LaCrAsO	$P4/nmm$ (129)	P_c4_2/ncm (138.528)	$4/mmm1'$	×	×
1.147	$Li_2Fe(SO_4)_2$	$P2_1/c$ (14)	P_a2_1/c (14.80)	$2/m1'$	×	×
1.148	$CeOs_{1.84}Ir_{0.16}Al_{10}$	$Cmcm$ (63)	P_Anma (62.453)	$mmm1'$	×	×
1.149	$La_{0.8}Bi_{0.2}Mn_2O_5$	$Pbam$ (55)	P_cbam (55.361)	$mmm1'$	×	×
1.150	PrAg	$Pm\bar{3}m$ (221)	P_Bmna (53.334)	$mmm1'$	×	×
1.151	$Mn_{0.375}Co_{0.375}Fe_{0.25}$	$Fm\bar{3}m$ (225)	P_A2_1/c (14.83)	$2/m1'$	×	×
1.152	Ce_3NIn	$Pm\bar{3}m$ (221)	$P_C\bar{4}b2$ (117.305)	$\bar{4}2m1'$	G-wP	×
1.153	Mn_3GaC	$Pm\bar{3}m$ (221)	$R_I\bar{3}c$ (167.108)	$\bar{3}m1'$	×	×
1.154	$NaFeSi_2O_6$	$C2/c$ (15)	P_C2_1/c (14.84)	$2/m1'$	×	×
1.155	$LiFeSO_4F$	$P\bar{1}$ (2)	$P_S\bar{1}$ (2.7)	$\bar{1}1'$	×	×
1.156	$LaMn_3Cr_4O_{12}$	$Im\bar{3}$ (204)	R_I3 (146.12)	$31'$	G-wP	×
1.157	$FeF_3(H_2O)_2H_2O$	$P4/n$ (85)	P_b2_1/c (14.81)	$2/m1'$	×	×
1.158	$YMn_3Al_4O_{12}$	$Im\bar{3}$ (204)	P_Innm (58.404)	$mmm1'$	×	×
1.159	$Li_2Ni(WO_4)_2$	$P\bar{1}$ (2)	$P_S\bar{1}$ (2.7)	$\bar{1}1'$	×	×
1.160	UP	$Fm\bar{3}m$ (225)	P_I4/mnc (128.410)	$4/mmm1'$	×	×
1.161	$PrFe_3(BO_3)_4$	$R32$ (155)	R_I32 (155.48)	$321'$	G-woP	×
1.162	NdMg	$Pm\bar{3}m$ (221)	P_c4/mcc (124.360)	$4/mmm1'$	×	×
1.163	TmPdIn	$P\bar{6}2m$ (189)	$P_c\bar{6}$ (174.136)	$\bar{6}1'$	G-woP	×
1.164	Co_3TeO_6	$C2/c$ (15)	$P_S\bar{1}$ (2.7)	$\bar{1}1'$	×	×
1.165	Ni_3TeO_6	$R3$ (146)	R_I3 (146.12)	$31'$	G-woP	×
1.166	La_2LiOsO_6	$P2_1/n$ (14)	$P_S\bar{1}$ (2.7)	$\bar{1}1'$	×	×
1.167	NiS_2	$Pa\bar{3}$ (205)	$P_S\bar{1}$ (2.7)	$\bar{1}1'$	×	×

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TABLE S1 – continued from previous page

BCS-ID	Formula	Parent	MSG	MPG	SHG type	LMO
1.168	Sr_2CuTeO_6	$I4/m$ (87)	C_c2/c (15.90)	$2/m1'$	×	×
1.169	$CaCoGe_2O_6$	$C2/c$ (15)	P_C2_1/c (14.84)	$2/m1'$	×	×
1.170	$Tm_5Ni_2In_4$	$Pbam$ (55)	C_am (8.36)	$m1'$	G-wP	×
1.171	$Tb_2Fe_2Si_2C$	$C2/m$ (12)	C_c2/m (12.63)	$2/m1'$	×	×
1.172	$NiTa_2O_6$	$P4_2/mnm$ (136)	A_bba2 (41.217)	$mm21'$	G-wP	×
1.173	$La_{0.375}Ca_{0.625}MnO_3$	$Pnma$ (62)	P_bmc2_1 (26.72)	$mm21'$	G-wP	×
1.174	$La_{0.333}Ca_{0.667}MnO_3$	$Pnma$ (62)	P_bmc2_1 (26.72)	$mm21'$	G-wP	×
1.175	$La_{0.333}Ca_{0.667}MnO_3$	$Pbnm$ (62)	P_bmn2_1 (31.129)	$mm21'$	G-wP	×
1.176	$YbCo_2Si_2$	$I4/mmm$ (139)	I_cbca (73.553)	$mmm1'$	×	×
1.177	Sr_2CuWO_6	$I4/m$ (87)	$P_S\bar{1}$ (2.7)	$\bar{1}1'$	×	×
1.178	$Cu_{1.07}Mn_{0.93}O_2$	$C2/m$ (12)	$P_S\bar{1}$ (2.7)	$\bar{1}1'$	×	×
1.179	$NdCoAsO$	$P4/nmm$ (129)	P_anma (62.450)	$mmm1'$	×	×
1.180	$Na_3Co_2SbO_6$	$C2/m$ (12)	$P_S\bar{1}$ (2.7)	$\bar{1}1'$	×	×
1.181	$Ba_3Fe_3O_7F$	$P2_1/m$ (11)	P_a2_1/m (11.55)	$2/m1'$	×	×
1.182	$TlMnO_3$	$Pm\bar{3}m$ (221)	$P_S\bar{1}$ (2.7)	$\bar{1}1'$	×	×
1.183	$FePS_3$	$C2/m$ (12)	C_c2/m (12.63)	$2/m1'$	×	×
1.184	$Na_2Co_2TeO_6$	$P6_322$ (182)	$P_C2_12_12_1$ (19.29)	$2221'$	G-woP	×
1.185	$GeCu_2O_4$	$I4_1/amd$ (141)	$I_c\bar{4}2d$ (122.338)	$\bar{4}2m1'$	G-wP	×
1.186	$SrRu_2O_6$	$P\bar{3}1m$ (162)	$P_c\bar{3}1m$ (162.78)	$\bar{3}m1'$	×	×
1.187	$TbRh_2Si_2$	$I4/mmm$ (139)	P_I4/mnc (128.410)	$4/mmm1'$	×	×
1.188	$CeRh_2Si_2$	$I4/mmm$ (139)	C_Amca (64.480)	$mmm1'$	×	×
1.189	$TbMg_3$	$Fm\bar{3}m$ (225)	$R_I\bar{3}c$ (167.108)	$\bar{3}m1'$	×	×
1.190	$YCr(BO_3)_2$	$R\bar{3}$ (148)	$P_S\bar{1}$ (2.7)	$\bar{1}1'$	×	×
1.191	$HoCr(BO_3)_2$	$R\bar{3}$ (148)	$P_S\bar{1}$ (2.7)	$\bar{1}1'$	×	×
1.192	$SmMn_2O_5$	$Pbam$ (55)	P_bmc2_1 (26.72)	$mm21'$	G-wP	×
1.193	$CrTe_3$	$P2_1/c$ (14)	$P_S\bar{1}$ (2.7)	$\bar{1}1'$	×	×
1.194	$NiWO_4$	$P2/c$ (13)	P_a2/c (13.70)	$2/m1'$	×	×
1.195	Er_2Ni_2In	$Cmmm$ (65)	C_amcm (63.467)	$mmm1'$	×	×
1.196	MnV_2O_6	$Pbcn$ (60)	P_a2_1/c (14.80)	$2/m1'$	×	×
1.197	$Fe_4Si_2Sn_7O_{16}$	$P\bar{3}m1$ (164)	C_c2/m (12.63)	$2/m1'$	×	×
1.198	$Ni_{1.64}Co_{0.36}Mn_{1.28}Ga_{0.72}$	$I4/mmm$ (139)	P_I4_2/mnm (136.506)	$4/mmm1'$	×	×
1.199	Sc_2NiMnO_6	$P2_1/c$ (14)	P_a2_1/c (14.80)	$2/m1'$	×	×
1.200	U_2Ni_2Sn	$P4/mbm$ (127)	C_cmcm (63.466)	$mmm1'$	×	×
1.201	Cr_2ReO_6	$P4_2/mnm$ (136)	P_a2_1/c (14.80)	$2/m1'$	×	×
1.202	$CrReO_4$	$C2/m$ (12)	C_c2/c (15.90)	$2/m1'$	×	×
1.203	Ni_2SiO_4	$Pnma$ (62)	P_c2_1/c (14.82)	$2/m1'$	×	×
1.204	Ni_2SiO_4	$Pnma$ (62)	P_c2_1/c (14.82)	$2/m1'$	×	×
1.205	$Dy_2Fe_2Si_2C$	$C2/m$ (12)	C_c2/m (12.63)	$2/m1'$	×	×
1.206	$Dy_2Fe_2Si_2C$	$C2/m$ (12)	$P_S\bar{1}$ (2.7)	$\bar{1}1'$	×	×
1.207	U_2Rh_2Sn	$P4/mbm$ (127)	P_c4_2/mbc (135.492)	$4/mmm1'$	×	×
1.208	UAs	$Fm\bar{3}m$ (225)	P_I4/mnc (128.410)	$4/mmm1'$	×	×
1.209	FeI_2	$P\bar{3}m1$ (164)	C_c2/c (15.90)	$2/m1'$	×	×
1.210	$FePSe_3$	$R\bar{3}$ (148)	$P_S\bar{1}$ (2.7)	$\bar{1}1'$	×	×
1.211	Dy_2O_2S	$P\bar{3}m1$ (164)	C_c2/c (15.90)	$2/m1'$	×	×
1.212	Dy_2O_2Se	$P\bar{3}m1$ (164)	C_c2/c (15.90)	$2/m1'$	×	×
1.213	Ho_2O_2Se	$P\bar{3}m1$ (164)	P_A2/c (13.73)	$2/m1'$	×	×
1.214	Yb_2O_2Se	$P\bar{3}m1$ (164)	C_c2/c (15.90)	$2/m1'$	×	×
1.215	UP_2	$P4/nmm$ (129)	P_c4/ncc (130.432)	$4/mmm1'$	×	×
1.216	Nd_2BaNiO_5	$Immm$ (71)	C_c2/c (15.90)	$2/m1'$	×	×
1.217	Tb_2BaNiO_5	$Immm$ (71)	C_c2/c (15.90)	$2/m1'$	×	×
1.218	Tm_2BaNiO_5	$Immm$ (71)	$P_S\bar{1}$ (2.7)	$\bar{1}1'$	×	×
1.219	CuF_2	$P2_1/c$ (14)	$P_S\bar{1}$ (2.7)	$\bar{1}1'$	×	×
1.220	$YBa_2Fe_3O_{8.08}$	$P4/mmm$ (123)	I_bmma (74.562)	$mmm1'$	×	×
1.221	$YBa_2Fe_3O_{7.84}$	$Pmmm$ (47)	C_a2/m (12.64)	$2/m1'$	×	×
1.222	Er_2CoGa_8	$P4/mmm$ (123)	P_amma (51.298)	$mmm1'$	×	×
1.223	Tm_2CoGa_8	$P4/mmm$ (123)	C_ammm (65.489)	$mmm1'$	×	×
1.224	$CoNb_2O_6$	$Pbcn$ (60)	$P_c2_12_12_1$ (19.28)	$2221'$	G-wP	×

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TABLE S1 – continued from previous page

BCS-ID	Formula	Parent	MSG	MPG	SHG type	LMO
1.225	$ScMn_6Ge_6$	$P6/mmm$ (191)	P_c6/mcc (192.252)	$6/mmm1'$	×	×
1.226	$CeCo_2Ge_4O_{12}$	$P4/nbm$ (125)	P_bnna (52.315)	$mmm1'$	×	×
1.227	$Ca_2Cr_2O_5$	$I2mb$ (46)	P_C2_1 (4.12)	$21'$	G-woP	×
1.228	$RuCl_3$	$C2/m$ (12)	P_C2/m (10.49)	$2/m1'$	×	×
1.229	$BaMoP_2O_8$	$C2/m$ (12)	$P_S\bar{1}$ (2.7)	$\bar{1}1'$	×	×
1.230	$NiPS_3$	$C2/m$ (12)	P_C2_1/m (11.57)	$2/m1'$	×	×
1.231	$NiPS_3$	$C2/m$ (12)	P_S1 (1.3)	$11'$	G-wP	×
1.232	$CuMnSb$	$F\bar{4}3m$ (216)	C_cc (9.40)	$m1'$	G-woP	×
1.233	$CuMnSb$	$F\bar{4}3m$ (216)	R_I3c (161.72)	$3m1'$	G-woP	×
1.234	$Ca_2Sr_2IrO_6$	$R\bar{3}$ (148)	$P_S\bar{1}$ (2.7)	$\bar{1}1'$	×	×
1.235	$Ba(TiO)Cu_4(PO_4)_4$	$P4_22_12$ (90)	P_c422_12 (94.132)	$4221'$	G-woP	×
1.236	$ErFeCuGe_4O_{12}$	$P4/nbm$ (125)	P_c4/nnc (126.384)	$4/mmm1'$	×	×
1.237	VCl_2	$P\bar{3}m1$ (164)	P_c31c (159.64)	$3m1'$	G-wP	×
1.238	VBr_2	$P\bar{3}m1$ (164)	P_c31c (159.64)	$3m1'$	G-wP	×
1.239	$MnBr_2$	$P\bar{3}m1$ (164)	C_c2/m (12.63)	$2/m1'$	×	×
1.240	FeI_2	$P\bar{3}m1$ (164)	$P_S\bar{1}$ (2.7)	$\bar{1}1'$	×	×
1.241	$FeCl_2$	$R\bar{3}m$ (166)	$R_I\bar{3}c$ (167.108)	$\bar{3}m1'$	×	×
1.242	$FeBr_2$	$P\bar{3}m1$ (164)	$P_c\bar{3}c1$ (165.96)	$\bar{3}m1'$	×	×
1.243	Sr_2CoOsO_6	$I2/m$ (12)	$P_S\bar{1}$ (2.7)	$\bar{1}1'$	×	×
1.244	$CrCl_3$	$R\bar{3}$ (148)	$P_S\bar{1}$ (2.7)	$\bar{1}1'$	×	×
1.245	$CoBr_2$	$P\bar{3}m1$ (164)	C_c2/c (15.90)	$2/m1'$	×	×
1.246	$CoCl_2$	$R\bar{3}m$ (166)	C_c2/c (15.90)	$2/m1'$	×	×
1.247	$NiCl_2$	$R\bar{3}m$ (166)	C_c2/c (15.90)	$2/m1'$	×	×
1.248	$NiBr_2$	$R\bar{3}m$ (166)	C_c2/c (15.90)	$2/m1'$	×	×
1.249	K_2NiF_4	$I4/mmm$ (139)	C_Amca (64.480)	$mmm1'$	×	×
1.250	$KNiF_3$	$Pm\bar{3}m$ (221)	I_c4/mcm (140.550)	$4/mmm1'$	×	×
1.251	$NdCo_2P_2$	$I4/mmm$ (139)	P_c4/mcc (124.360)	$4/mmm1'$	×	×
1.252	$CaCo_2P_2$	$I4/mmm$ (139)	P_Immn (59.416)	$mmm1'$	×	×
1.253	$CeCo_2P_2$	$I4/mmm$ (139)	P_I4/nnc (126.386)	$4/mmm1'$	×	×
1.254	$UNiGa_5$	$P4/mmm$ (123)	I_c4/mcm (140.550)	$4/mmm1'$	×	×
1.255	$UPtGa_5$	$P4/mmm$ (123)	P_c4/mcc (124.360)	$4/mmm1'$	×	×
1.256	$BaNi_2V_2O_8$	$R\bar{3}$ (148)	$P_S\bar{1}$ (2.7)	$\bar{1}1'$	×	×
1.257	$BaNi_2As_2O_8$	$R\bar{3}$ (148)	$P_S\bar{1}$ (2.7)	$\bar{1}1'$	×	×
1.258	$Cu_3Co_2SbO_6$	$C2/c$ (15)	P_C2_1/c (14.84)	$2/m1'$	×	×
1.259	$Cu_3Ni_2SbO_6$	$C2/c$ (15)	P_C2/c (13.74)	$2/m1'$	×	×
1.260	$NaMnGe_2O_6$	$C2/c$ (15)	$P_S\bar{1}$ (2.7)	$\bar{1}1'$	×	×
1.261	$NpRhGa_5$	$P4/mmm$ (123)	P_c4/mcc (124.360)	$4/mmm1'$	×	×
1.262	$NpRhGa_5$	$P4/mmm$ (123)	C_cmcm (63.466)	$mmm1'$	×	×
1.263	$Ca_3Ru_2O_7$	$Bb2_1m$ (36)	P_Cna2_1 (33.154)	$mm21'$	G-woP	×
1.264	$CoPS_3$	$C2/m$ (12)	P_C2_1/m (11.57)	$2/m1'$	×	×
1.265	$CuMnSb$	$F\bar{4}3m$ (216)	R_I3c (161.72)	$3m1'$	G-woP	×
1.266	$SmFe_3(BO_3)_4$	$R32$ (155)	P_S1 (1.3)	$11'$	G-woP	×
1.267	$Dy_2Co_3Al_9$	$Cmcm$ (63)	A_amm2 (38.192)	$mm21'$	G-wP	×
1.268	$Fe_{0.48}TiSe_2$	$I2/m$ (12)	C_c2/c (15.90)	$2/m1'$	×	×
1.269	$Fe_{0.48}TiSe_2$	$I2/m$ (12)	C_c2/c (15.90)	$2/m1'$	×	×
1.270	$Fe_{0.25}TiSe_2$	$F2/m$ (12)	C_c2/c (15.90)	$2/m1'$	×	×
1.271	$CeSbTe$	$P4/nmm$ (129)	P_c4/ncc (130.432)	$4/mmm1'$	×	×
1.272	$CeNiAsO$	$P4/nmm$ (129)	P_a2_1 (4.10)	$21'$	G-wP	×
1.273	$Pr_{0.5}Sr_{0.5}MnO_3$	$I4/mcm$ (140)	C_Amcm (63.468)	$mmm1'$	×	×
1.274	$DyFeWO_6$	$Pna2_1$ (33)	C_ac (9.41)	$m1'$	G-woP	×
1.275	$Ba_6Co_6ClO_{15.5}$	$P\bar{6}m2$ (187)	$P_c\bar{6}c2$ (188.220)	$\bar{6}m21'$	G-woP	×
1.276	$Na_{0.5}Li_{0.5}FeGe_2O_6$	$P2_1/c$ (14)	P_a2_1/c (14.80)	$2/m1'$	×	×
1.277	$LiFeCr_4O_8$	$F\bar{4}3m$ (216)	$I\bar{4}m'2'$ (119.319)	$\bar{4}2'm'$	BW-woP	✓
1.278	$Cu(NCS)_2$	$P\bar{1}$ (2)	$P_S\bar{1}$ (2.7)	$\bar{1}1'$	×	×
1.279	$Ho_2Cu_2O_5$	$Pna2_1$ (33)	P_a2_1 (4.10)	$21'$	G-woP	×
1.280	$Yb_2Cu_2O_5$	$Pna2_1$ (33)	P_ac (7.27)	$m1'$	G-woP	×
1.281	$YBaCuFeO_5$	$P4mm$ (99)	F_Smm2 (42.223)	$mm21'$	G-woP	×

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TABLE S1 – continued from previous page

BCS-ID	Formula	Parent	MSG	MPG	SHG type	LMO
1.282	$YBaCuFeO_5$	$P4/mmm$ (123)	C_a2/m (12.64)	$2/m1'$	×	×
1.283	$YBaCuFeO_5$	$P4/mmm$ (123)	C_a2/m (12.64)	$2/m1'$	×	×
1.284	$YBaCuFeO_5$	$P4/mmm$ (123)	C_a2/m (12.64)	$2/m1'$	×	×
1.285	$YBaCuFeO_5$	$P4/mmm$ (123)	F_Smmm (69.526)	$mmm1'$	×	×
1.286	$Fe_2(C_2O_4)_{3.4}H_2O$	$P\bar{1}$ (2)	$P_S\bar{1}$ (2.7)	$\bar{1}1'$	×	×
1.287	V_2O_3	$I2/a$ (15)	P_C2_1/c (14.84)	$2/m1'$	×	×
1.288	$CePd_2Si_2$	$I4/mmm$ (139)	C_Accm (66.5)	$mmm1'$	×	×
1.289	$CePd_2Ge_2$	$I4/mmm$ (139)	C_Accm (66.5)	$mmm1'$	×	×
1.290	$CeRh_2Si_2$	$I4/mmm$ (139)	C_Amca (64.480)	$mmm1'$	×	×
1.291	$CeAu_2Si_2$	$I4/mmm$ (139)	P_I4/mnc (128.410)	$4/mmm1'$	×	×
1.292	$HoNi_2B_2C$	$I4/mmm$ (139)	C_Amca (64.480)	$mmm1'$	×	×
1.293	$NdNi_2B_2C$	$I4/mmm$ (139)	C_c2/c (15.90)	$2/m1'$	×	×
1.294	$HoNi_2B_2C$	$I4/mmm$ (139)	C_Amca (64.480)	$mmm1'$	×	×
1.295	$DyNi_2B_2C$	$I4/mmm$ (139)	C_Amca (64.480)	$mmm1'$	×	×
1.296	$PrNi_2B_2C$	$I4/mmm$ (139)	C_Amca (64.480)	$mmm1'$	×	×
1.297	$CuFe_2(P_2O_7)_2$	$P2_1/n$ (14)	P_a2_1/c (14.80)	$2/m1'$	×	×
1.298	$BaCdVO(PO_4)_2$	$Pbca$ (61)	P_bna2_1 (33.150)	$mm21'$	G-wP	×
1.299	$GdMn_2O_5$	$Pbam$ (55)	P_aca2_1 (29.104)	$mm21'$	G-wP	×
1.300	$GdMn_2O_5$	$Pbam$ (55)	P_aca2_1 (29.104)	$mm21'$	G-wP	×
1.301	$BiMnTeO_6$	$P2_1/c$ (14)	P_a2_1/c (14.80)	$2/m1'$	×	×
1.302	Ba_2CoO_4	$P2_1/n$ (14)	P_a2_1/c (14.80)	$2/m1'$	×	×
1.303	$Dy_3Ru_4Al_{12}$	$P6_3/mmc$ (194)	C_c2/c (15.90)	$2/m1'$	×	×
1.304	$ZnMnO_3$	$R\bar{3}$ (148)	$P_S\bar{1}$ (2.7)	$\bar{1}1'$	×	×
1.305	Mn_5Si_3	$P6_3/mcm$ (193)	P_Cbcn (60.431)	$mmm1'$	×	×
1.306	$Na_2BaMn(VO_4)_2$	$C2/c$ (15)	P_C2_1/c (14.84)	$2/m1'$	×	×
1.307	Mn_5Si_3	$P6_3/mcm$ (193)	P_S1 (1.3)	$11'$	G-wP	×
1.308	$MnBi_2Te_4$	$R\bar{3}m$ (166)	$R_I\bar{3}c$ (167.108)	$\bar{3}m1'$	×	×
1.309	$MnBi_2Te_4$	$R\bar{3}m$ (166)	$R_I\bar{3}c$ (167.108)	$\bar{3}m1'$	×	×
1.310	$MnBi_4Te_7$	$P\bar{3}m1$ (164)	$P_c\bar{3}c1$ (165.96)	$\bar{3}m1'$	×	×
1.311	$BaMo(PO_4)_2$	$C2/m$ (12)	$P_S\bar{1}$ (2.7)	$\bar{1}1'$	×	×
1.312	$HoNi_2B_2C$	$I4/mmm$ (139)	C_Amca (64.480)	$mmm1'$	×	×
1.313	$GdFeZnGe_4O_{12}$	$P4/nbm$ (125)	P_bnna (52.315)	$mmm1'$	×	×
1.314	$NaFeSi_2O_6$	$C2/c$ (15)	P_C2_1/c (14.84)	$2/m1'$	×	×
1.315	$Mn_{0.81}Cu_{0.19}WO_4$	$P2/c$ (13)	P_a2/c (13.70)	$2/m1'$	×	×
1.316	$La_{0.25}Pr_{0.75}Co_2P_2$	$I4/mmm$ (139)	P_c4/mcc (124.360)	$4/mmm1'$	×	×
1.317	$La_{0.25}Pr_{0.75}Co_2P_2$	$I4/mmm$ (139)	C_c2/c (15.90)	$2/m1'$	×	×
1.318	$Sr_2Ru_{0.95}Fe_{0.05}O_4$	$I4/mmm$ (139)	C_cmca (64.478)	$mmm1'$	×	×
1.319	$Sr_2Ru_{0.95}Fe_{0.05}O_4$	$I4/mmm$ (139)	C_cmcm (63.466)	$mmm1'$	×	×
1.320	Sr_2FeWO_6	$P2_1/n$ (14)	$P_S\bar{1}$ (2.7)	$\bar{1}1'$	×	×
1.321	Ba_2FeWO_6	$I4/m$ (87)	$P_S\bar{1}$ (2.7)	$\bar{1}1'$	×	×
1.322	Sr_2FeWO_5N	$I4/m$ (87)	$P_S\bar{1}$ (2.7)	$\bar{1}1'$	×	×
1.323	$CoGeO_3$	$C2/c$ (15)	P_C2_1/c (14.84)	$2/m1'$	×	×
1.324	$DyMn_2O_5$	$Pbam$ (55)	P_aca2_1 (29.104)	$mm21'$	G-wP	×
1.325	$PrMn_2O_5$	$Pbam$ (55)	P_cc (7.28)	$m1'$	G-wP	×
1.326	$PrMn_2O_5$	$Pbam$ (55)	P_bnma (62.451)	$mmm1'$	×	×
1.327	$LaMn_2O_5$	$Pbam$ (55)	P_cbam (55.361)	$mmm1'$	×	×
1.328	Yb_2CoMnO_6	$P2_1/c$ (14)	P_a2_1 (4.10)	$21'$	G-wP	×
1.329	$YbLuCoMnO_6$	$P2_1/c$ (14)	P_a2_1 (4.10)	$21'$	G-wP	×
1.330	Lu_2CoMnO_6	$P2_1/c$ (14)	P_a2_1 (4.10)	$21'$	G-wP	×
1.331	$Li_{0.31}Na_{0.69}FeGe_2O_6$	$P2_1/c$ (14)	P_a2_1/c (14.80)	$2/m1'$	×	×
1.332	$Li_{0.22}Na_{0.78}FeGe_2O_6$	$C2/c$ (15)	P_C2_1/c (14.84)	$2/m1'$	×	×
1.333	$Yb_2Pd_2(In_{0.4}Sn_{0.6})$	$P4/mbm$ (127)	P_c4/mbm (127.396)	$4/mmm1'$	×	×
1.334	Pr_2Pd_2In	$P4/mbm$ (127)	P_bnma (62.451)	$mmm1'$	×	×
1.335	Nd_2Pd_2In	$P4/mbm$ (127)	P_cmc2_1 (26.73)	$mm21'$	G-wP	×
1.336	$Tb_2Pd_{2.05}Sn_{0.95}$	$P4/mbm$ (127)	P_bnma (62.451)	$mmm1'$	×	×
1.337	$U_2Pd_{2.35}Sn_{0.65}$	$P4/mbm$ (127)	P_c4/mnc (128.408)	$4/mmm1'$	×	×
1.338	U_2Ni_2In	$P4/mbm$ (127)	P_c4/mnc (128.408)	$4/mmm1'$	×	×
1.339	$EuAs_3$	$C2/m$ (12)	C_c2/m (12.63)	$2/m1'$	×	×

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TABLE S1 – continued from previous page

BCS-ID	Formula	Parent	MSG	MPG	SHG type	LMO
1.340	$LuMnO_3$	$Pbnm$ (62)	P_bmn2_1 (31.129)	$mm21'$	G-wP	×
1.341	$TmMnO_3$	$Pnma$ (62)	P_bmn2_1 (31.129)	$mm21'$	G-wP	×
1.342	$Co_3(PO_4)_2$	$P2_1/c$ (14)	P_a2_1/c (14.80)	$2/m1'$	×	×
1.343	$Ba_2Co_9O_{14}$	$R\bar{3}m$ (166)	C_c2/c (15.90)	$2/m1'$	×	×
1.344	$Ba_2Co_9O_{14}$	$R\bar{3}m$ (166)	C_c2/m (12.63)	$2/m1'$	×	×
1.345	$NaMnF_4$	$P2_1/c$ (14)	P_a2_1/c (14.80)	$2/m1'$	×	×
1.346	$TlMnF_4$	$I2/a$ (15)	P_C2/c (13.74)	$2/m1'$	×	×
1.347	$CuFeO_2$	$R\bar{3}m$ (166)	C_a2/c (15.91)	$2/m1'$	×	×
1.348	$CuFeO_2$	$R\bar{3}m$ (166)	C_c2/c (15.90)	$2/m1'$	×	×
1.349	$CoNb_3S_6$	$P6_322$ (182)	$P_B2_12_12$ (18.22)	$2221'$	G-woP	×
1.350	Nd_2BaCoO_5	$Immm$ (71)	C_c2/c (15.90)	$2/m1'$	×	×
1.351	$Ba_2Co_2F_7Cl$	$P2_1/m$ (11)	P_a2_1/m (11.55)	$2/m1'$	×	×
1.352	$Ba_2Ni_2F_7Cl$	$P2_1/m$ (11)	P_c2_1/c (14.82)	$2/m1'$	×	×
1.353	$SmNiO_3$	$Pnma$ (62)	C_amc2_1 (36.178)	$mm21'$	G-wP	×
1.354	$EuNiO_3$	$Pnma$ (62)	C_amc2_1 (36.178)	$mm21'$	G-wP	×
1.355	$DyGe_3$	$Cmcm$ (63)	P_a2_1/m (11.55)	$2/m1'$	×	×
1.356	Ho_3Ge_4	$Cmcm$ (63)	P_Bnna (52.318)	$mmm1'$	×	×
1.357	Ho_3Ge_4	$Cmcm$ (63)	P_c2_1/c (14.82)	$2/m1'$	×	×
1.358	$HoGe_{1.5}$	$P6/mmm$ (191)	C_cmcm (63.466)	$mmm1'$	×	×
1.359	Dy_3Ge_4	$Cmcm$ (63)	P_a2_1/m (11.55)	$2/m1'$	×	×
1.360	$DyGe_{1.3}$	$P6/mmm$ (191)	C_cmcm (63.466)	$mmm1'$	×	×
1.361	$DyGe$	$Cmcm$ (63)	C_c2/c (15.90)	$2/m1'$	×	×
1.362	Er_3Ge_4	$Cmcm$ (63)	P_Cbcm (57.391)	$mmm1'$	×	×
1.363	$TbCu_2Si_2$	$I4/mmm$ (139)	$P_S\bar{1}$ (2.7)	$\bar{1}1'$	×	×
1.364	$HoCu_2Si_2$	$I4/mmm$ (139)	$P_S\bar{1}$ (2.7)	$\bar{1}1'$	×	×
1.365	$TbCu_2Si_2$	$I4/mmm$ (139)	$P_S\bar{1}$ (2.7)	$\bar{1}1'$	×	×
1.366	$HoCu_2Si_2$	$I4/mmm$ (139)	C_c2/m (12.63)	$2/m1'$	×	×
1.367	Pu_2O_3	$P\bar{3}m1$ (164)	C_c2/c (15.90)	$2/m1'$	×	×
1.368	$Tb_2Ni_3Si_5$	$Ibam$ (72)	P_Ibam (55.364)	$mmm1'$	×	×
1.369	HFe_2Ge_2	$I4/mmm$ (139)	C_Amca (64.480)	$mmm1'$	×	×
1.370	Li_2CuO_2	$Immm$ (71)	P_Innm (58.404)	$mmm1'$	×	×
1.371	Nd_2NiO_4	$Cmce$ (64)	P_Cmna (53.335)	$mmm1'$	×	×
1.372	$Sr_2MnO_2Ag_{1.5}Se_2$	$I4/mmm$ (139)	P_I4/mnc (128.410)	$4/mmm1'$	×	×
1.373	$Li_3Ni_2SbO_6$	$C2/m$ (12)	$P_S\bar{1}$ (2.7)	$\bar{1}1'$	×	×
1.374	$HoNiGe$	$Pnma$ (62)	P_cc (7.28)	$m1'$	G-wP	×
1.375	$CeScGe$	$I4/mmm$ (139)	$P_S\bar{1}$ (2.7)	$\bar{1}1'$	×	×
1.376	$CeScGe$	$I4/mmm$ (139)	C_Amcm (63.468)	$mmm1'$	×	×
1.377	$CeScSi$	$I4/mmm$ (139)	$P_S\bar{1}$ (2.7)	$\bar{1}1'$	×	×
1.378	$CeScSi$	$I4/mmm$ (139)	C_Amcm (63.468)	$mmm1'$	×	×
1.379	$ErNiGe$	$Pnma$ (62)	P_a2_1/c (14.80)	$2/m1'$	×	×
1.380	Sr_2FeO_3Cl	$P4/nmm$ (129)	$P_C\bar{4}2_1m$ (113.273)	$\bar{4}2m1'$	G-wP	×
1.381	Sr_2FeO_3Br	$P4/nmm$ (129)	$P_C\bar{4}2_1m$ (113.273)	$\bar{4}2m1'$	G-wP	×
1.382	Ca_2FeO_3Cl	$P4/nmm$ (129)	$P_C\bar{4}2_1m$ (113.273)	$\bar{4}2m1'$	G-wP	×
1.383	Ca_2FeO_3Br	$P4/nmm$ (129)	$P_C\bar{4}2_1m$ (113.273)	$\bar{4}2m1'$	G-wP	×
1.384	USb_2	$P4/nmm$ (129)	P_c4/ncc (130.432)	$4/mmm1'$	×	×
1.385	Sr_2FeO_3F	$P4/nmm$ (129)	$P_C\bar{4}2_1m$ (113.273)	$\bar{4}2m1'$	G-wP	×
1.386	Sr_2FeO_3F	$P4/nmm$ (129)	$I_c\bar{4}2m$ (121.332)	$\bar{4}2m1'$	G-wP	×
1.387	Sr_2FeO_3F	$P4/nmm$ (129)	$P_C\bar{4}2m$ (111.257)	$\bar{4}2m1'$	G-wP	×
1.388	$La_2NiO_3F_2$	$Cccm$ (66)	P_Amna (53.333)	$mmm1'$	×	×
1.389	Sr_2CoO_3Cl	$P4/nmm$ (129)	P_Bccm (49.274)	$mmm1'$	×	×
1.390	$La_2NiO_3F_{1.93}$	$C2/c$ (15)	P_C2_1/c (14.84)	$2/m1'$	×	×
1.391	Fe_2MnBO_5	$Pbam$ (55)	P_bnma (62.451)	$mmm1'$	×	×
1.392	$KCuMnS_2$	$I4/mmm$ (139)	C_Ammm (65.490)	$mmm1'$	×	×
1.393	$Pb_2BaCuFeO_5Br$	$P4/mmm$ (123)	I_bmma (74.562)	$mmm1'$	×	×
1.394	$Pb_2BaCuFeO_5Cl$	$P4/mmm$ (123)	I_bmma (74.562)	$mmm1'$	×	×
1.395	$NdCeBaCuFeO_7$	$I4/mmm$ (139)	C_Accm (66.5)	$mmm1'$	×	×
1.396	$NdCeBaCu_{0.9}Co_{1.1}O_7$	$I4/mmm$ (139)	C_Amca (64.480)	$mmm1'$	×	×

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BCS-ID	Formula	Parent	MSG	MPG	SHG type	LMO
1.397	$Cu_3Mg(OD)_6Br_2$	$P\bar{3}m1$ (164)	C_c2/m (12.63)	$2/m1'$	×	×
1.398	Pr_2CuO_4	$I4/mmm$ (139)	C_Accm (66.5)	$mmm1'$	×	×
1.399	Pr_2CuO_4	$I4/mmm$ (139)	C_Accm (66.5)	$mmm1'$	×	×
1.400	$TbAg_2$	$I4/mmm$ (139)	C_Amca (64.480)	$mmm1'$	×	×
1.401	Nd_5Pb_3	$P6_3/mcm$ (193)	P_Bnma (62.454)	$mmm1'$	×	×
1.402	Nd_5Pb_3	$P6_3/mcm$ (193)	P_Bnma (62.454)	$mmm1'$	×	×
1.403	La_2CoO_4	$Cmce$ (64)	P_Cmna (53.335)	$mmm1'$	×	×
1.404	$Sr_2CuO_2Cl_2$	$I4/mmm$ (139)	C_Amca (64.480)	$mmm1'$	×	×
1.405	La_2CuO_4	$Bmeb$ (64)	P_Accn (56.374)	$mmm1'$	×	×
1.406	Nd_2CuO_4	$I4/mmm$ (139)	C_Accm (66.5)	$mmm1'$	×	×
1.407	Nd_2CuO_4	$I4/mmm$ (139)	C_Amca (64.480)	$mmm1'$	×	×
1.408	Nd_2CuO_4	$I4/mmm$ (139)	C_Accm (66.5)	$mmm1'$	×	×
1.409	$NaMnO_2$	$C2/m$ (12)	$P_S\bar{1}$ (2.7)	$\bar{1}1'$	×	×
1.410	$Sr_2Fe_{1.9}Cr_{0.1}O_5$	$Icmm$ (74)	P_Imna (53.336)	$mmm1'$	×	×
1.411	$EuMn_2P_2$	$P\bar{3}m1$ (164)	C_c2/m (12.63)	$2/m1'$	×	×
1.412	$Au_{72}Al_{14}Tb_{14}$	$Im\bar{3}$ (204)	$P_In\bar{3}$ (201.21)	$m\bar{3}1'$	×	×
1.413	$Ce_3Ni_2Ge_7$	$Cmmm$ (65)	P_Cmmn (59.415)	$mmm1'$	×	×
1.414	$CeNiGe_3$	$Cmmm$ (65)	P_Cmmn (59.415)	$mmm1'$	×	×
1.415	Tb_2Pd_2In	$P4/mbm$ (127)	C_amca (64.479)	$mmm1'$	×	×
1.416	Tb_2O_2S	$P\bar{3}m1$ (164)	C_c2/c (15.90)	$2/m1'$	×	×
1.417	Tb_2O_2Se	$P\bar{3}m1$ (164)	C_c2/c (15.90)	$2/m1'$	×	×
1.418	Cu_4O_3	$I4_1/amd$ (141)	$I_c\bar{4}2m$ (121.332)	$\bar{4}2m1'$	G-wP	×
1.419	$GdIn_3$	$Pm\bar{3}m$ (221)	P_C4/mbm (127.397)	$4/mmm1'$	×	×
1.420	$YBa_2Cu_3O_6$	$P4/mmm$ (123)	C_ammm (65.489)	$mmm1'$	×	×
1.421	$NdRh_2Si_2$	$I4/mmm$ (139)	P_I4/mnc (128.410)	$4/mmm1'$	×	×
1.422	$ErRh_2Si_2$	$I4/mmm$ (139)	P_Inmm (58.404)	$mmm1'$	×	×
1.423	UPb_3	$Pm\bar{3}m$ (221)	P_c4/mcc (124.360)	$4/mmm1'$	×	×
1.424	UCu_5	$F\bar{4}3m$ (216)	R_I3c (161.72)	$3m1'$	G-woP	×
1.425	$UGeTe$	$I4/mmm$ (139)	P_I4/nnc (126.386)	$4/mmm1'$	×	×
1.426	$UGeS$	$P4/nmm$ (129)	P_c4/ncc (130.432)	$4/mmm1'$	×	×
1.427	$HoCo_2Ge_2$	$I4/mmm$ (139)	P_I4/mnc (128.410)	$4/mmm1'$	×	×
1.428	UN	$Fm\bar{3}m$ (225)	P_I4/mnc (128.410)	$4/mmm1'$	×	×
1.429	$BaFe_2Se_3$	$Pnma$ (62)	C_am (8.36)	$m1'$	G-wP	×
1.430	$Mn_5(VO_4)_2(OH)_4$	$C2/m$ (12)	P_b2/c (13.71)	$2/m1'$	×	×
1.431	$Ca_2Mn_3O_8$	$C2/m$ (12)	$P_S\bar{1}$ (2.7)	$\bar{1}1'$	×	×
1.432	Ba_2LuRuO_6	$Fm\bar{3}m$ (225)	C_Amca (64.480)	$mmm1'$	×	×
1.433	Ba_2YRuO_6	$Fm\bar{3}m$ (225)	C_Amca (64.480)	$mmm1'$	×	×
1.434	$Fe_{1.05}Te$	$P4/nmm$ (129)	P_a2_1/m (11.55)	$2/m1'$	×	×
1.435	$Fe_{1.05}Te$	$P4/nmm$ (129)	P_a2_1/m (11.55)	$2/m1'$	×	×
1.436	$Fe_{1.125}Te$	$P4/nmm$ (129)	$P_S\bar{1}$ (2.7)	$\bar{1}1'$	×	×
1.437	$Fe_{1.068}Te$	$P4/nmm$ (129)	$P_S\bar{1}$ (2.7)	$\bar{1}1'$	×	×
1.438	$BaCoF_4$	$A2_1am$ (36)	P_a2_1 (4.10)	$21'$	G-woP	×
1.439	$BaCoF_4$	$A2_1am$ (36)	P_bca2_1 (29.105)	$mm21'$	G-woP	×
1.440	$CrPS_4$	$C2$ (5)	C_c2 (5.16)	$21'$	G-woP	×
1.441	$NaFe_3(SO_4)_2(OH)_6$	$R\bar{3}m$ (166)	$R_I\bar{3}c$ (167.108)	$\bar{3}m1'$	×	×
1.442	URu_2Si_2	$I4/mmm$ (139)	P_I4/mnc (128.410)	$4/mmm1'$	×	×
1.443	Gd_2BaCuO_5	$Pnma$ (62)	P_aca2_1 (29.104)	$mm21'$	G-wP	×
1.444	Er_2Pt	$Pnma$ (62)	P_ana2_1 (33.149)	$mm21'$	G-wP	×
1.445	Y_2BaCuO_5	$Pnma$ (62)	P_a2_1/c (14.80)	$2/m1'$	×	×
1.446	$CeCoAl_4$	$Pmma$ (51)	C_amca (64.479)	$mmm1'$	×	×
1.447	$Ce_3Ni_2Sn_7$	$Cmmm$ (65)	P_Cmmn (59.415)	$mmm1'$	×	×
1.448	$HoSi$	$Cmcm$ (63)	C_a2/c (15.91)	$2/m1'$	×	×
1.449	$Li_2CuW_2O_8$	$P\bar{1}$ (2)	$P_S\bar{1}$ (2.7)	$\bar{1}1'$	×	×
1.450	$Pr_6Fe_{13}Sn$	$I4/mcm$ (140)	P_Ibcn (60.432)	$mmm1'$	×	×
1.451	$Nd_6Fe_{13}Sn$	$I4/mcm$ (140)	P_I4/mcc (124.362)	$4/mmm1'$	×	×
1.452	$FeSn$	$P6/mmm$ (191)	C_cmcm (63.466)	$mmm1'$	×	×
1.453	$EuMn_2Si_2$	$I4/mmm$ (139)	P_I4/nnc (126.386)	$4/mmm1'$	×	×

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BCS-ID	Formula	Parent	MSG	MPG	SHG type	LMO
1.454	$Mn_6Ni_{16}Si_7$	$Fm\bar{3}m$ (225)	C_Amca (64.480)	$mmm1'$	×	×
1.455	$Mn_6Ni_{16}Si_7$	$Fm\bar{3}m$ (225)	P_A2_1/c (14.83)	$2/m1'$	×	×
1.456	$Sr_2CuO_2Cu_2S_2$	$I4/mmm$ (139)	$I_c\bar{4}2d$ (122.338)	$\bar{4}2m1'$	G-wP	×
1.457	$NdNiMg_{15}$	$P4/nmm$ (129)	P_Bcca (54.350)	$mmm1'$	×	×
1.458	$CsCo_2Se_2$	$I4/mmm$ (139)	C_Amcm (63.468)	$mmm1'$	×	×
1.459	$CeFe_3(BO_3)_4$	$R32$ (155)	C_c2 (5.16)	$21'$	G-woP	×
1.460	PrCuSi	$P6_3/mmc$ (194)	P_Cbcn (60.431)	$mmm1'$	×	×
1.461	$Sr_2Cr_3As_2O_2$	$I4/mmm$ (139)	P_I4_2/mnm (136.506)	$4/mmm1'$	×	×
1.462	La_2CoPtO_6	$P2_1/n$ (14)	P_a2_1/c (14.80)	$2/m1'$	×	×
1.463	$Sr_2Fe_3Se_2O_3$	$Pbam$ (55)	C_amc2_1 (36.178)	$mm21'$	G-wP	×
1.464	U_2N_2P	$P\bar{3}m1$ (164)	$P_c\bar{3}c1$ (165.96)	$\bar{3}m1'$	×	×
1.465	U_2N_2As	$P\bar{3}m1$ (164)	$P_c\bar{3}c1$ (165.96)	$\bar{3}m1'$	×	×
1.466	$MnPt_{0.5}Pd_{0.5}$	$P4/mmm$ (123)	C_amma (67.509)	$mmm1'$	×	×
1.467	$Tb_{0.6}Y_{0.4}RhIn_5$	$P4/mmm$ (123)	C_amma (67.509)	$mmm1'$	×	×
1.468	$TbMn_2Si_2$	$I4/mmm$ (139)	P_I4/nnc (126.386)	$4/mmm1'$	×	×
1.469	YMn_2Si_2	$I4/mmm$ (139)	P_I4/nnc (126.386)	$4/mmm1'$	×	×
1.470	UCr_2Si_2	$C2/m$ (12)	C_c2/c (15.90)	$2/m1'$	×	×
1.471	$EuCd_2As_2$	$P\bar{3}m1$ (164)	C_c2/m (12.63)	$2/m1'$	×	×
1.472	CaOFeS	$P6_3mc$ (186)	P_Cca2_1 (29.109)	$mm21'$	G-woP	×
1.473	$CuBr(C_4H_4N_2)_2(BF_4)$	$P4/nbm$ (125)	P_bnna (52.315)	$mmm1'$	×	×
1.474	$CuCl(C_4H_4N_2)_2(BF_4)$	$P4/nbm$ (125)	P_bnna (52.315)	$mmm1'$	×	×
1.475	$DyNiAl_4$	$Cmcm$ (63)	P_Anma (62.453)	$mmm1'$	×	×
1.476	Ba_2CoO_4	$P2_1/n$ (14)	P_a2_1/c (14.80)	$2/m1'$	×	×
1.477	Ba_2CoO_4	$P2_1/n$ (14)	P_a2_1/c (14.80)	$2/m1'$	×	×
1.478	$CoTi_2O_5$	$Cmcm$ (63)	P_a2_1/m (11.55)	$2/m1'$	×	×
1.479	U_2Ni_2Sn	$P4/mbm$ (127)	P_c4_2/mbc (135.492)	$4/mmm1'$	×	×
1.480	Mn_2CoReO_6	$P2_1/n$ (14)	$P_S\bar{1}$ (2.7)	$\bar{1}1'$	×	×
1.481	$LaSr_3Fe_3O_9$	$Cmcm$ (63)	P_Cbcm (57.391)	$mmm1'$	×	×
1.482	$Er_2Fe_2Si_2C$	$C2/m$ (12)	$P_S\bar{1}$ (2.7)	$\bar{1}1'$	×	×
1.483	$Eu_{0.5}Ca_{0.5}Fe_2As_2$	$Fmmm$ (69)	C_Amca (64.480)	$mmm1'$	×	×
1.484	Li_2MnGeO_4	$Pmn2_1$ (31)	C_ac (9.41)	$m1'$	G-woP	×
1.485	Mn_3TeO_6	$P2_1/c$ (14)	P_a2_1/c (14.80)	$2/m1'$	×	×
1.486	$CeRhAl_4Si_2$	$P4/mmm$ (123)	P_c4/mcc (124.360)	$4/mmm1'$	×	×
1.487	$CeIrAl_4Si_2$	$P4/mmm$ (123)	P_c4/mcc (124.360)	$4/mmm1'$	×	×
1.488	$CeMn_2Si_2$	$I4/mmm$ (139)	P_I4/nnc (126.386)	$4/mmm1'$	×	×
1.489	$CeMn_2Si_2$	$I4/mmm$ (139)	P_I4/nnc (126.386)	$4/mmm1'$	×	×
1.490	$CeMn_2Si_2$	$I4/mmm$ (139)	P_I4/nnc (126.386)	$4/mmm1'$	×	×
1.491	$PrMn_2Si_2$	$I4/mmm$ (139)	P_I4/nnc (126.386)	$4/mmm1'$	×	×
1.492	$PrMn_2Si_2$	$I4/mmm$ (139)	P_I4/nnc (126.386)	$4/mmm1'$	×	×
1.493	$NdMn_2Si_2$	$I4/mmm$ (139)	P_I4/nnc (126.386)	$4/mmm1'$	×	×
1.494	$NdMn_2Si_2$	$I4/mmm$ (139)	P_I4/nnc (126.386)	$4/mmm1'$	×	×
1.495	YMn_2Si_2	$I4/mmm$ (139)	P_I4/nnc (126.386)	$4/mmm1'$	×	×
1.496	YMn_2Ge_2	$I4/mmm$ (139)	P_I4/nnc (126.386)	$4/mmm1'$	×	×
1.497	$EuMg_2Bi_2$	$P\bar{3}m1$ (164)	C_c2/m (12.63)	$2/m1'$	×	×
1.498	$Cu_6(SiO_3)_6(H_2O)_6$	$R\bar{3}$ (148)	$R_I\bar{3}$ (148.20)	$\bar{3}1'$	×	×
1.499	$CsFe(MoO_4)_2$	$P\bar{3}$ (147)	P_c3 (143.3)	$31'$	G-wP	×
1.500	$Sr_2CoO_2Cu_2S_2$	$I4/mmm$ (139)	$P_S\bar{1}$ (2.7)	$\bar{1}1'$	×	×
1.501	$Ba_2CoO_2Cu_2S_2$	$I4/mmm$ (139)	$P_S\bar{1}$ (2.7)	$\bar{1}1'$	×	×
1.502	$Li_3Co_2SbO_6$	$C2/m$ (12)	C_c2/m (12.63)	$2/m1'$	×	×
1.503	$NdScSiC_{0.5}H_{0.2}$	$I4/mmm$ (139)	P_I4/nnc (126.386)	$4/mmm1'$	×	×
1.504	GdCuSn	$P6_3mc$ (186)	P_Cna2_1 (33.154)	$mm21'$	G-woP	×
1.505	GdAgSn	$P6_3mc$ (186)	P_Cna2_1 (33.154)	$mm21'$	G-woP	×
1.506	GdAuSn	$P6_3mc$ (186)	P_Cna2_1 (33.154)	$mm21'$	G-woP	×
1.507	$NdPd_5Al_2$	$I4/mmm$ (139)	P_anma (62.450)	$mmm1'$	×	×
1.508	Mn_2AlB_2	$Cmmm$ (65)	C_cmcm (63.466)	$mmm1'$	×	×
1.509	$Pd_{2.87}Mn_{0.88}$	$I4/mmm$ (139)	P_A2_1/c (14.83)	$2/m1'$	×	×
1.510	$TbNi_2Ge_2$	$I4/mmm$ (139)	P_c4/mcc (124.360)	$4/mmm1'$	×	×
1.511	$TbNi_2Si_2$	$I4/mmm$ (139)	C_Amca (64.480)	$mmm1'$	×	×

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TABLE S1 – continued from previous page

BCS-ID	Formula	Parent	MSG	MPG	SHG type	LMO
1.512	$TbCo_2Si_2$	$I4/mmm$ (139)	P_I4/mnc (128.410)	$4/mmm1'$	×	×
1.513	$HoCo_2Si_2$	$I4/mmm$ (139)	P_I4/mnc (128.410)	$4/mmm1'$	×	×
1.514	$HoCo_2Si_2$	$I4/mmm$ (139)	P_I4/mnc (128.410)	$4/mmm1'$	×	×
1.515	$ErCo_2Si_2$	$I4/mmm$ (139)	P_A2_1/c (14.83)	$2/m1'$	×	×
1.516	$ErCo_2Si_2$	$I4/mmm$ (139)	P_Innm (58.404)	$mmm1'$	×	×
1.517	$DyBe_{13}$	$Fm\bar{3}c$ (226)	C_A222_1 (20.37)	$2221'$	G-wP	×
1.518	$TbBe_{13}$	$Fm\bar{3}c$ (226)	C_A222_1 (20.37)	$2221'$	G-wP	×
1.519	$CoSO_4$	$Cmcm$ (63)	P_Cbcn (60.431)	$mmm1'$	×	×
1.520	$NiSO_4$	$Cmcm$ (63)	P_Cbcn (60.431)	$mmm1'$	×	×
1.521	$FeSO_4$	$Cmcm$ (63)	P_Cbcn (60.431)	$mmm1'$	×	×
1.522	$CrVO_4$	$Cmcm$ (63)	$P\bar{1}$ (2.4)	$\bar{1}$	×	✓
1.523	VPO_4	$Cmcm$ (63)	P_cnma (62.452)	$mmm1'$	×	×
1.524	$InMnO_3$	$P6_3cm$ (185)	P_c31c (159.64)	$3m1'$	G-woP	×
1.525	$InMnO_3$	$P6_3cm$ (185)	P_c31m (157.56)	$3m1'$	G-woP	×
1.526	$LiCoF_4$	$P2_1/c$ (14)	P_a2_1/c (14.80)	$2/m1'$	×	×
1.527	$CsNiF_3$	$P6_3/mmc$ (194)	P_Bnnm (58.402)	$mmm1'$	×	×
1.528	$Bi_2Fe_4O_9$	$Pbam$ (55)	C_a2/m (12.64)	$2/m1'$	×	×
1.529	$MnBi_6Te10$	$R\bar{3}m$ (166)	$R_I\bar{3}c$ (167.108)	$\bar{3}m1'$	×	×
1.530	CeC_2	$I4/mmm$ (139)	P_I4/mnc (128.410)	$4/mmm1'$	×	×
1.531	PrC_2	$I4/mmm$ (139)	P_I4/mnc (128.410)	$4/mmm1'$	×	×
1.532	NdC_2	$I4/mmm$ (139)	P_I4/mnc (128.410)	$4/mmm1'$	×	×
1.533	TbC_2	$I4/mmm$ (139)	P_c222_1 (17.12)	$2221'$	G-wP	×
1.534	HoC_2	$I4/mmm$ (139)	P_amma (51.298)	$mmm1'$	×	×
1.535	UPd_2Ge_2	$I4/mmm$ (139)	P_c4/ncc (130.432)	$4/mmm1'$	×	×
1.536	UPd_2Si_2	$I4/mmm$ (139)	P_I4/mnc (128.410)	$4/mmm1'$	×	×
1.537	URh_2Si_2	$I4/mmm$ (139)	P_I4/mnc (128.410)	$4/mmm1'$	×	×
1.538	Ba_2MnTeO_6	$R\bar{3}m$ (166)	P_A2_1/c (14.83)	$2/m1'$	×	×
1.539	KMnP	$P4/nmm$ (129)	P_c4_2/ncm (138.528)	$4/mmm1'$	×	×
1.540	KMnP	$P4/nmm$ (129)	P_c4_2/ncm (138.528)	$4/mmm1'$	×	×
1.541	RbMnP	$P4/nmm$ (129)	P_c4_2/ncm (138.528)	$4/mmm1'$	×	×
1.542	RbMnP	$P4/nmm$ (129)	P_c4_2/ncm (138.528)	$4/mmm1'$	×	×
1.543	RbMnAs	$P4/nmm$ (129)	P_c4_2/ncm (138.528)	$4/mmm1'$	×	×
1.544	RbMnAs	$P4/nmm$ (129)	P_c4_2/ncm (138.528)	$4/mmm1'$	×	×
1.545	RbMnBi	$P4/nmm$ (129)	P_c4_2/ncm (138.528)	$4/mmm1'$	×	×
1.546	CsMnBi	$P4/nmm$ (129)	P_c4_2/ncm (138.528)	$4/mmm1'$	×	×
1.547	CsMnP	$P4/nmm$ (129)	P_c4_2/ncm (138.528)	$4/mmm1'$	×	×
1.548	CsMnP	$P4/nmm$ (129)	P_c4_2/ncm (138.528)	$4/mmm1'$	×	×
1.549	U_2Ni_2In	$P4/mbm$ (127)	P_c4/mnc (128.408)	$4/mmm1'$	×	×
1.550	LiMnAs	$P4/nmm$ (129)	P_c4_2/ncm (138.528)	$4/mmm1'$	×	×
1.551	LiMnAs	$P4/nmm$ (129)	P_c4_2/ncm (138.528)	$4/mmm1'$	×	×
1.552	LiMnAs	$P4/nmm$ (129)	P_c4_2/ncm (138.528)	$4/mmm1'$	×	×
1.553	KMnAs	$P4/nmm$ (129)	P_c4_2/ncm (138.528)	$4/mmm1'$	×	×
1.554	KMnAs	$P4/nmm$ (129)	P_c4_2/ncm (138.528)	$4/mmm1'$	×	×
1.555	Mn_3B_4	$Immm$ (71)	P_Innm (58.404)	$mmm1'$	×	×
1.556	$FeSn_2$	$I4/mcm$ (140)	P_Ibcn (60.432)	$mmm1'$	×	×
1.557	$FeGe_2$	$I4/mcm$ (140)	P_Ibcn (60.432)	$mmm1'$	×	×
1.558	$MnSn_2$	$I4/mcm$ (140)	C_Acca (68.520)	$mmm1'$	×	×
1.559	$MnSn_2$	$I4/mcm$ (140)	C_cccm (66.498)	$mmm1'$	×	×
1.560	$GeNi_2O_4$	$Fd\bar{3}m$ (227)	C_c2/m (12.63)	$2/m1'$	×	×
1.561	$GeNi_2O_4$	$Fd\bar{3}m$ (227)	C_cm (8.35)	$m1'$	G-wP	×
1.562	$GeNi_2O_4$	$Fd\bar{3}m$ (227)	C_c2 (5.16)	$21'$	G-wP	×
1.563	$GeNi_2O_4$	$Fd\bar{3}m$ (227)	C_cm (8.35)	$m1'$	G-wP	×
1.564	$GeCo_2O_4$	$Fd\bar{3}m$ (227)	C_c2 (5.16)	$21'$	G-wP	×
1.565	Pb_2CoOsO_6	$P2_1/n$ (14)	P_ac (7.27)	$m1'$	G-wP	×
1.566	Ba_2YbRuO_6	$Fm\bar{3}m$ (225)	P_I4/mnc (128.410)	$4/mmm1'$	×	×
1.567	Ba_2TmRuO_6	$Fm\bar{3}m$ (225)	P_I4/mnc (128.410)	$4/mmm1'$	×	×
1.568	$GdCu_2Si_2$	$I4/mmm$ (139)	C_c2/m (12.63)	$2/m1'$	×	×

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TABLE S1 – continued from previous page

BCS-ID	Formula	Parent	MSG	MPG	SHG type	LMO
1.569	$SrRu_2O_6$	$P\bar{3}1m$ (162)	$P_c\bar{3}1m$ (162.78)	$\bar{3}m1'$	×	×
1.570	La_3OsO_7	$Cmcm$ (63)	P_a2_1/m (11.55)	$2/m1'$	×	×
1.571	La_3OsO_7	$Cmcm$ (63)	P_a2_1/m (11.55)	$2/m1'$	×	×
1.572	$La_{2.8}Ca_{0.2}OsO_7$	$Cmcm$ (63)	P_a2_1/m (11.55)	$2/m1'$	×	×
1.573	$FeSO_4$	$Pbnm$ (62)	P_c2_1/c (14.82)	$2/m1'$	×	×
1.574	NdBiPt	$F\bar{4}3m$ (216)	$P_I\bar{4}n2$ (118.314)	$\bar{4}2m1'$	G-woP	×
1.575	ErRh	$Pm\bar{3}m$ (221)	P_ammma (51.298)	$mmm1'$	×	×
1.576	Yb_2O_2S	$P\bar{3}m1$ (164)	C_c2/m (12.63)	$2/m1'$	×	×
1.577	$SrNd_2O_4$	$Pnam$ (62)	P_a2_1/c (14.80)	$2/m1'$	×	×
1.578	$KErSe_2$	$R\bar{3}m$ (166)	C_c2/m (12.63)	$2/m1'$	×	×
1.579	$NiTiO_3$	$R\bar{3}$ (148)	$P_S\bar{1}$ (2.7)	$\bar{1}1'$	×	×
1.580	$NiTiO_3$	$R\bar{3}$ (148)	$P_S\bar{1}$ (2.7)	$\bar{1}1'$	×	×
1.581	$FeTiO_3$	$R\bar{3}$ (148)	$R_I\bar{3}$ (148.20)	$\bar{3}1'$	×	×
1.582	$Fe_{0.945}O$	$Fm\bar{3}m$ (225)	$R_I\bar{3}c$ (167.108)	$\bar{3}m1'$	×	×
1.583	$La_{1.5}Ca_{0.5}CoO_4$	$Cmm2$ (35)	P_cc (7.28)	$m1'$	G-woP	×
1.584	PrFeAsO	$Cmme$ (67)	P_Bcca (54.350)	$mmm1'$	×	×
1.585	PrFeAsO	$Cmme$ (67)	P_Bcca (54.350)	$mmm1'$	×	×
1.586	PrFeAsO	$Cmme$ (67)	P_Acc2 (27.85)	$mm21'$	G-wP	×
1.587	NdFeAsO	$Cmme$ (67)	P_A2/c (13.73)	$2/m1'$	×	×
1.588	NdFeAsO	$Cmme$ (67)	I_cbca (73.553)	$mmm1'$	×	×
1.589	$Fe_{0.967}Nb_3S_6$	$P6_322$ (182)	$P_c2_12_12$ (18.21)	$2221'$	G-woP	×
1.590	$Pb_{0.8}Bi_{0.2}Fe_{0.728}WP_{0.264}O_8$	$Pm\bar{3}n$ (221)	I_c4/mcm (140.550)	$4/mmm1'$	×	×
1.591	$Pb_{0.7}Bi_{0.3}Fe_{0.762}WP_{0.238}O_8$	$Pm\bar{3}n$ (221)	I_c4/mcm (140.550)	$4/mmm1'$	×	×
1.592	Pb_2NiOsO_6	$P2_1/n$ (14)	P_ac (7.27)	$m1'$	G-wP	×
1.593	BaCoSO	$Cmcm$ (63)	P_abcm (57.386)	$mmm1'$	×	×
1.594	BaCoSO	$Cmcm$ (63)	P_abcm (57.386)	$mmm1'$	×	×
1.595	CaCoSO	$P6_3mc$ (186)	C_cc (9.40)	$m1'$	G-woP	×
1.596	$TbCuSb_2$	$P4/nmm$ (129)	$P_S\bar{1}$ (2.7)	$\bar{1}1'$	×	×
1.597	$TbCuSb_2$	$P4/nmm$ (129)	P_a2_1/m (11.55)	$2/m1'$	×	×
1.598	$CeIr(In_{0.97}Cd_{0.03})_5$	$P4/mmm$ (123)	I_c4/mcm (140.550)	$4/mmm1'$	×	×
1.599	$DyMn_2O_5$	$Pbam$ (55)	P_cc (7.28)	$m1'$	G-wP	×
1.600	$Bi_4Fe_5O_{13}F$	$P4_2/mbc$ (135)	P_C42/n (86.73)	$4/m1'$	×	×
1.601	$Bi_4Fe_5O_{13}F$	$P4_2/mbc$ (135)	P_C42/n (86.73)	$4/m1'$	×	×
1.602	$Bi_4Fe_5O_{13}F$	$P4_2/mbc$ (135)	P_C42/n (86.73)	$4/m1'$	×	×
1.603	$Bi_4Fe_5O_{13}F$	$P4_2/mbc$ (135)	P_C42/n (86.73)	$4/m1'$	×	×
1.604	$Bi_4Fe_5O_{13}F$	$P4_2/mbc$ (135)	P_C42/n (86.73)	$4/m1'$	×	×
1.605	$Bi_4Fe_5O_{13}F$	$P4_2/mbc$ (135)	P_C42/n (86.73)	$4/m1'$	×	×
1.606	$Bi_4Fe_5O_{13}F$	$P4_2/mbc$ (135)	P_C42/n (86.73)	$4/m1'$	×	×
1.607	$Bi_4Fe_5O_{13}F$	$P4_2/mbc$ (135)	P_C42/n (86.73)	$4/m1'$	×	×
1.608	$Bi_4Fe_5O_{13}F$	$P4_2/mbc$ (135)	P_C42/n (86.73)	$4/m1'$	×	×
1.609	$Bi_4Fe_5O_{13}F$	$P4_2/mbc$ (135)	P_C42/n (86.73)	$4/m1'$	×	×
1.610	$Bi_4Fe_5O_{13}F$	$P4_2/mbc$ (135)	P_C42/n (86.73)	$4/m1'$	×	×
1.611	$Bi_4Fe_5O_{13}F$	$P4_2/mbc$ (135)	P_C42/n (86.73)	$4/m1'$	×	×
1.612	$Bi_4Fe_5O_{13}F$	$P4_2/mbc$ (135)	P_C42/n (86.73)	$4/m1'$	×	×
1.613	$Bi_4Fe_5O_{13}F$	$P4_2/mbc$ (135)	P_C42/n (86.73)	$4/m1'$	×	×
1.614	$Bi_4Fe_5O_{13}F$	$P4_2/mbc$ (135)	P_C42/n (86.73)	$4/m1'$	×	×
1.615	$Bi_4Fe_5O_{13}F$	$P4_2/mbc$ (135)	P_C42/n (86.73)	$4/m1'$	×	×
1.616	$Bi_4Fe_5O_{13}F$	$P4_2/mbc$ (135)	P_C42/n (86.73)	$4/m1'$	×	×
1.617	$LiFe(MoO_4)_2$	$P\bar{1}$ (2)	$P_S\bar{1}$ (2.7)	$\bar{1}1'$	×	×
1.618	CoO	$Fm\bar{3}m$ (225)	C_c2/c (15.90)	$2/m1'$	×	×
1.619	MnS	$Fm\bar{3}m$ (225)	C_c2/m (12.63)	$2/m1'$	×	×
1.620	$NdCu_2$	$Imma$ (74)	P_Inma (62.456)	$mmm1'$	×	×
1.621	$La(Fe_{0.91}Al_{0.09})_{13}$	$Fm\bar{3}c$ (226)	P_I4/mcc (124.362)	$4/mmm1'$	×	×
1.622	$CoGeO_3$	$C2/c$ (15)	P_C2_1/c (14.84)	$2/m1'$	×	×
1.623	$EuMg_2Bi_2$	$P\bar{3}m1$ (164)	C_c2/m (12.63)	$2/m1'$	×	×
1.624	$EuSn_2P_2$	$R\bar{3}m$ (166)	C_c2/m (12.63)	$2/m1'$	×	×
1.625	$Sr_2Fe_3S_2O_3$	$Pbam$ (55)	P_bnma (62.451)	$mmm1'$	×	×

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TABLE S1 – continued from previous page

BCS-ID	Formula	Parent	MSG	MPG	SHG type	LMO
1.626	$Sr_2Fe_3Se_2O_3$	$Pbam$ (55)	C_amc2_1 (36.178)	$mm21'$	G-wP	×
1.627	$KCeS_2$	$R\bar{3}m$ (166)	C_c2/c (15.90)	$2/m1'$	×	×
1.628	$PrMnSi_2$	$Cmcm$ (63)	P_Bnna (52.318)	$mmm1'$	×	×
1.629	FeGe	$P6/mmm$ (191)	P_c6/mcc (192.252)	$6/mmm1'$	×	×
1.630	$LuMn_6Sn_6$	$P6/mmm$ (191)	C_cmcm (63.466)	$mmm1'$	×	×
1.631	YMn_6Ge_6	$P6/mmm$ (191)	P_c6/mcc (192.252)	$6/mmm1'$	×	×
1.632	$ErFe_6Ge_6$	$Immm$ (71)	P_Innn (48.264)	$mmm1'$	×	×
1.633	YFe_6Sn_6	$Immm$ (71)	P_Innn (48.264)	$mmm1'$	×	×
1.634	YFe_6Ge_6	$Cmcm$ (63)	P_Bnna (52.318)	$mmm1'$	×	×
1.635	$ErFe_2Si_2$	$I4/mmm$ (139)	P_anma (62.450)	$mmm1'$	×	×
1.636	$ErMn_2Si_2$	$I4/mmm$ (139)	P_I4/nnc (126.386)	$4/mmm1'$	×	×
1.637	$ErMn_2Si_2$	$I4/mmm$ (139)	P_I4/nnc (126.386)	$4/mmm1'$	×	×
1.638	$ErMn_2Ge_2$	$I4/mmm$ (139)	P_I4/nnc (126.386)	$4/mmm1'$	×	×
1.639	$ErMn_2Ge_2$	$I4/mmm$ (139)	P_I4/nnc (126.386)	$4/mmm1'$	×	×
1.640	$ErMn_2Ge_2$	$I4/mmm$ (139)	P_I4/nnc (126.386)	$4/mmm1'$	×	×
1.641	$Ba_2FeSi_2O_7$	$P\bar{4}2_1m$ (113)	C_cmc2_1 (36.177)	$mm21'$	G-woP	×
1.642	$TlFeS_2$	$C2/m$ (12)	C_c2/m (12.63)	$2/m1'$	×	×
1.643	DyOCl	$P4/nmm$ (129)	P_anma (62.450)	$mmm1'$	×	×
1.644	$EuSn_2As_2$	$R\bar{3}m$ (166)	C_c2/m (12.63)	$2/m1'$	×	×
1.645	$Na_2Co_2TeO_6$	$P6_322$ (182)	$P_C2_12_12_1$ (19.29)	$2221'$	G-woP	×
1.646	$Na_2Ni_2TeO_6$	$P6_3/mcm$ (193)	I_amm2 (44.234)	$mm21'$	G-wP	×
1.647	$Na_{2.4}Ni_2TeO_6$	$P6_3/mcm$ (193)	P_Anma (62.453)	$mmm1'$	×	×
1.648	Nd_2O_3	$P\bar{3}m1$ (164)	C_c2/m (12.63)	$2/m1'$	×	×
1.649	Sr_3ZnIrO_6	$R\bar{3}c$ (167)	P_C2/c (13.74)	$2/m1'$	×	×
1.650	$DyBaCuO_5$	$Pnma$ (62)	P_a2_1/c (14.80)	$2/m1'$	×	×
1.651	$HoBaCuO_5$	$Pnma$ (62)	P_a2_1/c (14.80)	$2/m1'$	×	×
1.652	$Tb_2Ni_{1.78}In$	$P/4mbm$ (127)	C_amca (64.479)	$mmm1'$	×	×
1.653	$FeWO_4$	$P2/c$ (13)	P_a2/c (13.70)	$2/m1'$	×	×
1.654	$NiNb_2O_6$	$Pbcn$ (60)	P_b2_1/c (14.81)	$2/m1'$	×	×
1.655	$FeNb_2O_6$	$Pbcn$ (60)	$P_c2_12_12_1$ (19.28)	$2221'$	G-wP	×
1.656	$CoNb_2O_6$	$Pbcn$ (60)	P_a2_1/c (14.80)	$2/m1'$	×	×
1.657	$LuNiO_3$	$P2_1/n$ (14)	P_a2_1 (4.10)	$21'$	G-wP	×
1.658	$DyGa_3$	$R\bar{3}m$ (166)	C_c2/c (15.90)	$2/m1'$	×	×
1.659	$MnCl_2(CO(NH_2)_2)_2$	$Ibca$ (45)	P_Ica2_1 (29.110)	$mm21'$	G-woP	×
1.660	$FePb_4Sb_6S_{14}$	$P2_1/c$ (14)	P_a2_1/c (14.80)	$2/m1'$	×	×
1.661	La_2NiIrO_6	$P2_1/n$ (14)	$P_S\bar{1}$ (2.7)	$\bar{1}1'$	×	×
1.662	La_2NiIrO_6	$P2_1/n$ (14)	$P_S\bar{1}$ (2.7)	$\bar{1}1'$	×	×
1.663	Tb_2Ni_2In	$Cmmm$ (65)	C_a2/m (12.64)	$2/m1'$	×	×
2.1	$EuFe_2As_2$	$I4/mmm$ (139)	P_Cbca (61.439)	$mmm1'$	×	×
2.2	$Sr_2F_2Fe_2OS_2$	$I4/mmm$ (139)	C_a2/m (12.64)	$2/m1'$	×	×
2.3	$HoNiO_3$	$P2_1/n$ (14)	$P2_1$ (4.7)	2	O-wP	✓
2.4	$Eu(Fe_{0.82}Co_{0.18})As_2$	$I4/mmm$ (139)	$Cmm'm'$ (65.486)	$m'm'm$	×	✓
2.5	Mn_3CuN	$Pm\bar{3}m$ (221)	$P4/n$ (85.59)	$4/m$	×	✓
2.6	Nd_2CuO_4	$I4/mmm$ (139)	P_C4_2/nnm (134.481)	$4/mmm1'$	×	×
2.7	Sm_2CuO_4	$I4/mmm$ (139)	P_C4_2/ncm (138.529)	$4/mmm1'$	×	×
2.8	$SrHo_2O_4$	$Pnam$ (62)	$P2_1/c'$ (14.78)	$2/m'$	PT-wP	×
2.9	$Ca_3CuNi_2(PO_4)_4$	$C2/c$ (15)	C_a2/c (15.91)	$2/m1'$	×	×
2.1	HoP	$Fm\bar{3}m$ (225)	$C2'/c'$ (15.89)	$2'/m'$	×	✓
2.11	TbMg	$Pm\bar{3}m$ (221)	$Pmm'a'$ (51.295)	$m'm'm$	×	✓
2.12	TbMg	$Pm\bar{3}m$ (221)	$Pc'cm'$ (49.270)	$m'm'm$	×	✓
2.13	UP	$Fm\bar{3}m$ (225)	P_C4_2/nnm (134.481)	$4/mmm1'$	×	×
2.14	NdMg	$Pm\bar{3}m$ (221)	P_C4/nbm (125.373)	$4/mmm1'$	×	×
2.15	$Mn_3Ni_20P_6$	$Fm\bar{3}m$ (225)	$Cmm'm'$ (65.486)	$m'm'm$	×	✓
2.16	Ce_2PdGe_3	$P4_2/mmc$ (131)	Pm' (6.20)	m'	BW-wP	✓
2.17	$Pb_2Mn_{0.6}Co_{0.4}WO_6$	$Pmcn$ (62)	$Pm'c2_1'$ (26.68)	$m'm2'$	BW-wP	✓
2.18	Sc_2NiMnO_6	$P2_1/c$ (14)	$P_S\bar{1}$ (2.7)	$\bar{1}1'$	×	×
2.19	Mn_3ZnC	$Pm\bar{3}m$ (221)	$I4/mm'm'$ (139.537)	$4/mm'm'$	×	✓

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BCS-ID	Formula	Parent	MSG	MPG	SHG type	LMO
2.20	UAs	$Fm\bar{3}m$ (225)	P_C4_2/nnm (134.481)	$4/mmm1'$	×	×
2.21	TbOOH	$P2_1/m$ (11)	$P2_1/c'$ (14.78)	$2/m'$	PT-wP	×
2.22	$FeTa_2O_6$	$P4_2/mnm$ (136)	I_c4_1/a (88.86)	$4/m1'$	×	×
2.23	$Sr_2CoO_2Ag_2Se_2$	$I4/mmm$ (139)	P_C42/n (86.73)	$4/m1'$	×	×
2.24	$Ba_2CoO_2Ag_2Se_2$	$I4/mmm$ (139)	P_C42/n (86.73)	$4/m1'$	×	×
2.25	Sr_2CoOsO_6	$I2/m$ (12)	$P_S\bar{1}$ (2.7)	$\bar{1}1'$	×	×
2.26	$PrCo_2P_2$	$I4/mmm$ (139)	$P4/mm'm'$ (123.345)	$4/mm'm'$	×	✓
2.27	$Sr_2Mn_3Sb_2O_2$	$I4/mmm$ (139)	$Cm'cm$ (63.459)	$m'mm$	PT-wP	×
2.28	$NpNiGa_5$	$P4/mmm$ (123)	$Imm'a'$ (74.559)	$m'm'm$	×	✓
2.29	Mn_3O_4	$I4_1/amd$ (141)	$Pb'c'n$ (60.422)	$m'm'm$	×	✓
2.30	$CeRh_2Si_2$	$I4/mmm$ (139)	P_Bcca (54.350)	$mmm1'$	×	×
2.31	Mn_3ZnN	$Pm\bar{3}m$ (221)	P_Ibcn (60.432)	$mmm1'$	×	×
2.32	$Dy_3Ru_4Al_{12}$	$P6_3/mmc$ (194)	$P\bar{3}c'1$ (165.95)	$\bar{3}m'$	×	✓
2.33	$Na_2Mn_3Se_4$	$C2/m$ (12)	$P_S\bar{1}$ (2.7)	$\bar{1}1'$	×	×
2.34	$La_{0.25}Pr_{0.75}Co_2P_2$	$I4/mmm$ (139)	$C2'/m'$ (12.62)	$2'/m'$	×	✓
2.35	CrSe	$P6_3/mmc$ (194)	$P31m'$ (157.55)	$3m'$	BW-wP	✓
2.36	$TbGe_3$	$Cmcm$ (63)	P_cnma (62.452)	$mmm1'$	×	×
2.37	$La_8Cu_7O_{19}$	$C2/c$ (15)	$P_S\bar{1}$ (2.7)	$\bar{1}1'$	×	×
2.38	Pb_2MnWO_6	$Pmc2_1$ (26)	$Pmn2_1$ (31.123)	$mm2$	O-woP	×
2.39	$LaCaFeO_4$	$I4/mmm$ (139)	P_C4_2/ncm (138.529)	$4/mmm1'$	×	×
2.40	$LaBaFeO_4$	$I4/mmm$ (139)	P_C4_2/ncm (138.529)	$4/mmm1'$	×	×
2.41	$LaSrFeO_4$	$I4/mmm$ (139)	P_C4_2/ncm (138.529)	$4/mmm1'$	×	×
2.42	$LaSrFeO_4$	$I4/mmm$ (139)	P_C4_2/nnm (134.481)	$4/mmm1'$	×	×
2.43	Fe_2MnBO_5	$Pbam$ (55)	$Pb'am'$ (55.358)	$m'm'm$	×	✓
2.44	$KCuMnS_2$	$I4/mmm$ (139)	P_C4/mmm (123.349)	$4/mmm1'$	×	×
2.45	$Pb_2BaCuFeO_5Br$	$P4/mmm$ (123)	P_C2 (3.6)	$21'$	G-wP	×
2.46	$Pb_2BaCuFeO_5Cl$	$P4/mmm$ (123)	P_C2 (3.6)	$21'$	G-wP	×
2.47	$Y_2SrCuFeO_{6.5}$	$Ibam$ (72)	$Pc'c'n$ (56.369)	$m'm'm$	×	✓
2.48	Pr_2CuO_4	$I4/mmm$ (139)	P_C4_2/nnm (134.481)	$4/mmm1'$	×	×
2.49	$La_2O_2Fe_2OSe_2$	$I4/mmm$ (139)	C_a2/m (12.64)	$2/m1'$	×	×
2.50	$EuMnBi_2$	$I4/mmm$ (139)	$P4_2'/m'm'c$ (131.440)	$4'/m'm'm$	PT-wP	×
2.51	$EuMnBi_2$	$I4/mmm$ (139)	$Pm'n'2_1$ (31.127)	$m'm'2$	BW-wP	✓
2.52	Mn_3O_4	$I4_1/amd$ (141)	Pc' (7.26)	m'	BW-wP	✓
2.53	$Ba_2Mn_3Sb_2O_2$	$I4/mmm$ (139)	$Cm'ma$ (67.503)	$m'mm$	PT-wP	×
2.54	$Sr_2Cr_3As_2O_2$	$I4/mmm$ (139)	P_C2_1/c (14.84)	$2/m1'$	×	×
2.55	$Sr_2Fe_3Se_2O_3$	$Pbam$ (55)	C_cc (9.40)	$m1'$	G-wP	×
2.56	$La_2O_2Fe_2OS_2$	$I4/mmm$ (139)	C_a2/m (12.64)	$2/m1'$	×	×
2.57	$TbMn_2Si_2$	$I4/mmm$ (139)	$Pmm'n'$ (59.410)	$m'm'm$	×	✓
2.58	$La_{0.73}Tb_{0.27}Mn_2Si_2$	$I4/mmm$ (139)	$Pnnm'$ (58.396)	$m'mm$	PT-wP	×
2.59	Mn_3As_2	$C2/m$ (12)	$C2/c$ (15.85)	$2/m$	×	✓
2.60	$NdMn_2Si_2$	$I4/mmm$ (139)	$Pmm'n'$ (59.410)	$m'm'm$	×	✓
2.61	$Fe_3F_8(H_2O)_2$	$C2/m$ (12)	$C2'/m'$ (12.62)	$2'/m'$	×	✓
2.62	$TbCrO_3$	$Pbnm$ (62)	$Pm'n'2_1$ (31.127)	$m'm'2$	BW-wP	✓
2.63	$DyCrO_3$	$Pbnm$ (62)	$P2_1'/m'$ (11.54)	$2'/m'$	×	✓
2.64	$DyCrO_3$	$Pbnm$ (62)	$P2_1'/m'$ (11.54)	$2'/m'$	×	✓
2.65	UPd_2Si_2	$I4/mmm$ (139)	$P4/mm'm'$ (123.345)	$4/mm'm'$	×	✓
2.66	$FeSn_2$	$I4/mcm$ (140)	$Cc'ca$ (68.513)	$m'mm$	PT-wP	×
2.67	$FeSn_2$	$I4/mcm$ (140)	P_Cbcn (60.431)	$mmm1'$	×	×
2.68	$FeGe_2$	$I4/mcm$ (140)	$Pc'cn$ (56.367)	$m'mm$	PT-wP	×
2.69	$La_{0.5}Ca_{0.5}MnO_3$	$Pnma$ (62)	P_a2_1/m (11.55)	$2/m1'$	×	×
2.70	GdMg	$Pm\bar{3}m$ (221)	$C2'/c'$ (15.89)	$2'/m'$	×	✓
2.71	HoRh	$Pm\bar{3}m$ (221)	P_C2_1/m (11.57)	$2/m1'$	×	×
2.72	VNb_3S_6	$P6_322$ (182)	$C2'2'2_1$ (20.33)	$2'2'2$	BW-woP	✓
2.73	$BaNd_2ZnO_5$	$I4/mcm$ (140)	P_C4/ncc (130.433)	$4/mmm1'$	×	×

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BCS-ID	Formula	Parent	MSG	MPG	SHG type	LMO
2.74	$BaDy_2O_4$	$Pnma$ (62)	$P2_1'$ (4.9)	$2'$	BW-wP	✓
2.75	$Sr_2Fe_3S_2O_3$	$Pbam$ (55)	P_A2_1/c (14.83)	$2/m1'$	×	×
2.76	$Sr_2Fe_3Se_2O_3$	$Pbam$ (55)	C_cc (9.40)	$m1'$	G-wP	×
2.77	Eu_2CuO_4	$I4/mmm$ (139)	P_C4_2/ncm (138.529)	$4/mmm1'$	×	×
2.78	Nd_2CuO_4	$I4/mmm$ (139)	P_C4_2/nnm (134.481)	$4/mmm1'$	×	×
2.79	Pr_2CuO_4	$I4/mmm$ (139)	P_C4_2/nnm (134.481)	$4/mmm1'$	×	×
2.80	$ErFe_6Ge_6$	$Immm$ (71)	$Pm'm'n$ (59.409)	$m'm'm$	×	✓
2.81	$ErMn_2Si_2$	$I4/mmm$ (139)	$Pm'm'n$ (59.409)	$m'm'm$	×	✓
2.82	$ErMn_2Si_2$	$I4/mmm$ (139)	$Pm'm'n$ (59.409)	$m'm'm$	×	✓
2.83	$ErMn_2Ge_2$	$I4/mmm$ (139)	$Pm'm'n$ (59.409)	$m'm'm$	×	✓
2.84	$ErMn_2Ge_2$	$I4/mmm$ (139)	$Pm'm'n$ (59.409)	$m'm'm$	×	✓
2.85	$HoBaCuO_5$	$Pnma$ (62)	$P2_1'/c$ (14.77)	$2'/m$	PT-wP	×
2.86	$FeTa_2O_6$	$P4_2/mnm$ (136)	I_c4_1/a (88.86)	$4/m1'$	×	×
3.1	TmAgGe	$P\bar{6}2m$ (189)	$P\bar{6}'2m'$ (189.224)	$\bar{6}'m'2$	BW-woP	×
3.2	UO_2	$Fm\bar{3}m$ (225)	$Pn\bar{3}m'$ (224.113)	$m\bar{3}m'$	×	×
3.3	Ho_2RhIn_8	$P4/mmm$ (123)	$Cm'cm'$ (63.464)	$m'm'm$	×	✓
3.4	$MgCr_2O_4$	$Fd\bar{3}m$ (227)	$P\bar{4}2'm'$ (111.255)	$\bar{4}2'm'$	BW-wP	✓
3.5	$Fe_{0.7}Mn_{0.3}$	$Fm\bar{3}m$ (225)	$Pn\bar{3}m'$ (224.113)	$m\bar{3}m'$	×	×
3.6	DyCu	$Pm\bar{3}m$ (221)	$Im\bar{3}m'$ (229.143)	$m\bar{3}m'$	×	×
3.7	NpBi	$Fm\bar{3}m$ (225)	$Pn\bar{3}m'$ (224.113)	$m\bar{3}m'$	×	×
3.8	NdZn	$Pm\bar{3}m$ (221)	$P_In\bar{3}n$ (222.103)	$m\bar{3}m1'$	×	×
3.9	NpS	$Fm\bar{3}m$ (225)	$F_Sd\bar{3}c$ (228.139)	$m\bar{3}m1'$	×	×
3.10	NpSe	$Fm\bar{3}m$ (225)	$F_Sd\bar{3}c$ (228.139)	$m\bar{3}m1'$	×	×
3.11	NpTe	$Fm\bar{3}m$ (225)	$F_Sd\bar{3}c$ (228.139)	$m\bar{3}m1'$	×	×
3.12	USb	$Fm\bar{3}m$ (225)	$Pn\bar{3}m'$ (224.113)	$m\bar{3}m'$	×	×
3.13	CeB_6	$Pm\bar{3}m$ (221)	C_amca (64.479)	$mmm1'$	×	×
3.14	FeI_2	$P\bar{3}m1$ (164)	$C2'/m'$ (12.62)	$2'/m'$	×	✓
3.15	FeI_2	$P\bar{3}m1$ (164)	$P\bar{3}m'1$ (164.89)	$\bar{3}m'$	×	✓
3.16	$Gd_2Ti_2O_7$	$Fd\bar{3}m$ (227)	$F_S\bar{4}3m$ (216.77)	$\bar{4}3m1'$	G-wP	×
3.17	$BaCu_3V_2O_8(OD)_2$	$P312_1$ (152)	$P312'1$ (152.35)	$32'$	BW-woP	✓
3.18	HoRh	$Pm\bar{3}m$ (221)	$P_Ia\bar{3}$ (205.36)	$m\bar{3}1'$	×	×
3.19	CoO	$Fm\bar{3}m$ (225)	I_c4_1/acd (142.570)	$4/mmm1'$	×	×