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# Comprehensive search for topological materials using symmetry indicators

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# Supplementary Information For “Comprehensive search for topological materials using symmetry indicators”

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## CONTENTS

I. Efficient topological materials screening	0
II. Towards ideal topological insulators and topological crystalline insulators	2
III. Topological (semi-)metals	5
IV. All of the predicted topological materials	9
V. AI basis vectors for 230 space groups	53
VI. Website for band structures	146
References	146

## I. EFFICIENT TOPOLOGICAL MATERIALS SCREENING

Our method of topological materials is based on the symmetry indicators [1], and it is highly efficient as we only need to calculate an expansion with respect to the atomic insulator basis (AIB). The 230 AIBs are explicitly shown for the 230 space groups ( $\mathcal{SG}$ s) in Sec. V of this supplementary material. As shown in Sec. V, each group owns a fixed number ( $d_{\text{AI}}$ ) of AIB vectors (denoted as  $a_i$ ) which are all integer-valued and may have a common factor (CF). We denote the CF of  $a_i$  by  $C_i$ . For the meaning of each row,  $\nu$  is the total number of the bands and  $n_{\mathbf{k},i}$  is the number of occurrences for the  $i$ th irreducible representation of the symmetry group of the high symmetry point  $\mathbf{k}$ . We arrange the AIB vectors, i.e.,  $a_1, a_2, \dots$  in the order of ascending CFs. The last AIB vector with the largest CF is the so-called strong AIB vector. In *ab initio* calculations, we only need to use the eigen-states at all the high symmetry points, and obtain  $n_{\mathbf{k},i}$  for the  $\nu_e$  bands ( $\nu_e$  is the total number of the valence electrons in the primitive unit cell). We thus obtain a vector  $\mathbf{n} = (\nu_e, n_{\mathbf{k}_1,1}, n_{\mathbf{k}_1,2}, \dots, n_{\mathbf{k}_2,1}, \dots)^{\top}$  and then we only need to compute a collection of expansion coefficients  $q_i$  [2]:

$$\mathbf{n} = \sum_i q_i a_i \equiv Aq \Rightarrow q = A^{-1}\mathbf{n}, \quad (1)$$

where the  $i$  column of  $A$  is just  $a_i$ , and  $A^{-1}$  denotes the pseudo-inverse of  $A$ . The topological property of the material can be diagnosed simply by inspecting the coefficients  $q_i$ . There are three cases: (1)  $q_i$  are all integers, implying the material could be an atomic insulator; (2) some  $q_i$  are fractions while  $q_i C_i$  are all integers, which implies all compatibility relations are satisfied and a continuous gap could be found at all high-symmetry points, lines, and planes; (3) Neither (1) nor (2) is true, which means there must be a band degeneracy at some high-symmetry points or lines.

Case (2) is the relevant case for the search of insulating topological materials. The possible sub-cases are:

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- (i) for centrosymmetric  $\mathcal{SG}$ s, let  $C_s$  be the largest CF and  $q_s$  be the expansion coefficient with respect to the corresponding AIB. Then if  $q_s C_s \bmod C_s$  is an odd number, we obtain a (strong) topological insulator (TI). Otherwise, we obtain a topological crystalline insulator (TCI);
- (ii) for  $S_4$  symmetric noncentrosymmetric  $\mathcal{SG}$ s one finds  $C_s = 2$ . For case 2,  $q_s C_s \bmod 2$  must be 1, which corresponds to a strong TI if it is not a Weyl semimetal (WSM);
- (iii) for  $C_3$  and mirror symmetric noncentrosymmetric  $\mathcal{SG}$ s with  $C_s = 3$ ,  $q_s C_s \bmod 3 = 1$  or 2 corresponds to a mirror Chern, strong and/ or a weak topological insulator if it is not a WSM.

Thus, from the CFs, we can assign an Abelian group  $X_{\text{BS}} = \mathbb{Z}_j \times \mathbb{Z}_{j+1} \times \dots \times \mathbb{Z}_{d_{\text{AI}}}$  where  $j$  denotes the first AIB vector whose CF is larger than 1. We use the results of  $r_m = q_m C_m \bmod C_m$  as the value in the factor group  $\mathbb{Z}_m$  where  $m = j, j+1, \dots, d_{\text{AI}}$ . They are written in the form of  $(r_j, r_{j+1}, \dots, r_{d_{\text{AI}}})$  which is called SI and can be used as a fast diagnosis of topological materials.

Note that, while a nonzero SI guarantees the existence of nontrivial band topology, generally it does not uniquely determine the precise topological phase of the system [1, 3]. Nonetheless, for almost all cases one can distinguish between a strong TI and a TCI using only the SI. The only exception to this concerns noncentrosymmetric  $\mathcal{SG}$ s with both a mirror together with a  $C_3$  rotation about the axis normal to the mirror plane (i.e., the  $\mathcal{SG}$  contains  $\bar{6}$  rotoinversion, but not  $C_6$  rotation), as we discussed above in the sub-case (iii) of case (2). Here is a complete list of such  $\mathcal{SG}$ s: **174**, **187**, **188**, **189**, and **190**. For these  $\mathcal{SG}$ s, materials listed in the table of TCIs might in fact be a strong TI. As an example, the strong TI AgAsCa [4] in  $\mathcal{SG}$  **189** has SI  $(1, 1) \in \mathbb{Z}_3 \times \mathbb{Z}_3$ , and is listed under Table II for TCIs.

## II. TOWARDS IDEAL TOPOLOGICAL INSULATORS AND TOPOLOGICAL CRYSTALLINE INSULATORS

We list all the relatively good topological insulators found in our search by GGA calculations in the following table. The structure references are provided after the names of these materials. Through a further checking by the MBJ calculations, if the GGA calculations predicted band topology is maintained, we print the material name in blue. While in some cases, the MBJ calculations, however, predict a TCI phase, we print the name in red. For the materials whose names are in black, the MBJ calculations mostly predict a trivial insulator though they are predicted as TIs by GGA calculations. In very few cases, the MBJ calculations predict a (semi-)metal phase.

Part 1 of Table I:

TABLE I. The list of 241 TIs with relatively clean Fermi surfaces discovered by GGA calculations: when the MBJ calculation doesn't change the band topology predicted by GGA calculations, we print the material in blue, while the red color means that the MBJ calculation results in a topological crystalline phase. Note that the elements in a compound are arranged in the alphabetical order, e.g., CaAs<sub>3</sub> is listed as As<sub>3</sub>Ca.

$\mathcal{S}\mathcal{G}$	$X_{\text{BS}}$	Topological insulators
<b>2</b>	$\mathbb{Z}_2^3 \times \mathbb{Z}_4$	Ag <sub>2</sub> F <sub>5</sub> [5], As <sub>3</sub> Ca[6, 7], As <sub>3</sub> Sr[8, 9], AgO <sub>4</sub> S[10], Br <sub>5</sub> W[11], CaMo <sub>6</sub> S <sub>8</sub> [12], CaP <sub>3</sub> [9, 13]
<b>11</b>	$\mathbb{Z}_2^2 \times \mathbb{Z}_4$	BBeLi[14], CaSb <sub>2</sub> [15], GeHfPd[16], HfS <sub>3</sub> [17], Mo <sub>2</sub> S <sub>3</sub> [18], Nb <sub>2</sub> Se <sub>3</sub> [19], Se <sub>3</sub> Ta <sub>2</sub> [19, 20]
<b>12</b>	$\mathbb{Z}_2^2 \times \mathbb{Z}_4$	Ag <sub>4</sub> K <sub>2</sub> Se <sub>3</sub> [21], Al <sub>2</sub> Ge <sub>4</sub> Sr <sub>3</sub> [22], Al <sub>8</sub> Mo <sub>3</sub> [23], As <sub>3</sub> Ba[9, 24], As <sub>3</sub> Sr[9, 25], Au <sub>2</sub> P <sub>3</sub> [26], BaSb <sub>3</sub> [27] Ba <sub>2</sub> Cd <sub>2</sub> Sb <sub>3</sub> [28], Ba <sub>2</sub> Hg <sub>3</sub> O <sub>14</sub> Pd <sub>7</sub> [29], Ba <sub>3</sub> Li <sub>4</sub> Sn <sub>8</sub> [30], BaTl <sub>4</sub> [31], Ba <sub>11</sub> Bi <sub>14</sub> Cds[32], Bi <sub>2</sub> Pb <sub>3</sub> S <sub>6</sub> [33] Bi <sub>4</sub> Pb <sub>7</sub> Se <sub>13</sub> [34], Br <sub>4</sub> Cs <sub>2</sub> I <sub>2</sub> Pd[35], Nb <sub>2</sub> PdS <sub>5</sub> [36], Nb <sub>2</sub> PdS <sub>6</sub> [37], Nb <sub>2</sub> PdSe <sub>6</sub> [37], P <sub>3</sub> Sr[38] , PdSe <sub>6</sub> Ta <sub>2</sub> [37], PtSe <sub>7</sub> Ta <sub>2</sub> [39]
<b>14</b>	$\mathbb{Z}_2 \times \mathbb{Z}_4$	Ag <sub>2</sub> Te[40, 41], AuI <sub>4</sub> Li[42], B <sub>2</sub> S <sub>3</sub> [43], BaNb <sub>2</sub> O <sub>6</sub> [44]
<b>15</b>	$\mathbb{Z}_2 \times \mathbb{Z}_4$	MoP <sub>4</sub> [45], O <sub>5</sub> Ti <sub>3</sub> [46]
<b>51</b>	$\mathbb{Z}_2^2 \times \mathbb{Z}_4$	AlPt <sub>2</sub> [47], AuITe <sub>2</sub> [48], Au <sub>3</sub> Rb <sub>2</sub> Tl[49]
<b>55</b>	$\mathbb{Z}_2 \times \mathbb{Z}_4$	Bi <sub>6</sub> In <sub>2</sub> Sr <sub>5</sub> [50]
<b>58</b>	$\mathbb{Z}_4$	Bi <sub>2</sub> Hf[51], S <sub>2</sub> Ti[52]
<b>59</b>	$\mathbb{Z}_2 \times \mathbb{Z}_4$	Ag <sub>3</sub> Sb[53], AuCs <sub>3</sub> Pb <sub>4</sub> [54], AuPb <sub>4</sub> Rb <sub>3</sub> [54], AuRb <sub>3</sub> Sn <sub>4</sub> [54]
<b>60</b>	$\mathbb{Z}_4$	Au <sub>2</sub> Pb[55], O <sub>2</sub> Pb[56]
<b>62</b>	$\mathbb{Z}_4$	AsCdNa[57], As <sub>2</sub> Hf[58], As <sub>2</sub> Zr[59, 60], Ba <sub>2</sub> Pb[61], Ba <sub>2</sub> Si[62, 63], Ca <sub>3</sub> GeO[64], CdGeSr[65], CdNaSb[66, 67], FSey[68] GeHfPt[69, 70], GeMoZr[71], GePdZr[72, 73], GePtZr[73, 74], GeZr[75], Ge <sub>2</sub> InLiSr <sub>2</sub> [76], Ge <sub>2</sub> Mo[77] Ge <sub>2</sub> W[78], HfNbP[79], HfP <sub>2</sub> [80], HfSi[81], NNa <sub>3</sub> [82], N <sub>5</sub> Ta <sub>3</sub> [83], PPtSc[73, 84] P <sub>2</sub> Zr[85], P <sub>2</sub> Ti[86], PbSr <sub>2</sub> [87, 88], PdSiTi[73, 89], PdSiZr[75], PtSiTi[73, 74], PtSiZr[73, 90], Sb <sub>2</sub> SrZn[91, 92], SiSr[93], SiTi[94], SiZr[94] AlLaPt[95], AuLa[95], GaLaPd[96], GaLaPt[96], GaLuPd[96], LaPPt[97]
<b>63</b>	$\mathbb{Z}_2 \times \mathbb{Z}_4$	AgS <sub>3</sub> Ta[98], AlBMo[99], AlBW[99], Al <sub>2</sub> BaSi <sub>2</sub> [100], AuClTe <sub>2</sub> [101], B <sub>7</sub> WY <sub>3</sub> [102], CaSi [103] Ga[104], GeNa <sub>2</sub> Zn[105], HfPd[106], HfTe <sub>5</sub> [107, 108], Te <sub>5</sub> Zr[107, 108] AlLa[109], GaLa[110], GaLu[111], LiLuSn <sub>2</sub> [112]
<b>64</b>	$\mathbb{Z}_2 \times \mathbb{Z}_4$	As[113], C <sub>2</sub> B <sub>2</sub> Mg[114]
<b>65</b>	$\mathbb{Z}_2^2 \times \mathbb{Z}_4$	Ag <sub>3</sub> Te <sub>2</sub> Tl[115], Ba <sub>3</sub> Ge <sub>4</sub> [116], AlB <sub>4</sub> Lu[117], LaSn <sub>2</sub> [118]
<b>69</b>	$\mathbb{Z}_2^2 \times \mathbb{Z}_4$	Be <sub>2</sub> Zn[119]
<b>71</b>	$\mathbb{Z}_2 \times \mathbb{Z}_4$	AsTeTi[120], Br <sub>2</sub> Ca <sub>3</sub> Si[121]
<b>72</b>	$\mathbb{Z}_2 \times \mathbb{Z}_4$	Br <sub>2</sub> Hg <sub>5</sub> O <sub>4</sub> [122]
<b>87</b>	$\mathbb{Z}_2 \times \mathbb{Z}_8$	Hf <sub>5</sub> Te <sub>4</sub> [123], Se <sub>4</sub> Ti <sub>5</sub> [124], Te <sub>4</sub> Zr <sub>5</sub> [125]
<b>121</b>	$\mathbb{Z}_2$	Ag <sub>2</sub> S <sub>4</sub> SnZn[126]
<b>122</b>	$\mathbb{Z}_2$	As <sub>2</sub> CdGe[127], As <sub>2</sub> CdSn[128], As <sub>2</sub> SnZn[129], CdSb <sub>2</sub> Sn[130]
<b>123</b>	$\mathbb{Z}_2 \times \mathbb{Z}_4 \times \mathbb{Z}_8$	BaGe <sub>3</sub> Mg <sub>4</sub> [131], ClNa <sub>2</sub> [132], ClNa <sub>3</sub> [132]
<b>127</b>	$\mathbb{Z}_4 \times \mathbb{Z}_8$	B <sub>4</sub> Y[133], CsI <sub>3</sub> Sn[134, 135], Pt <sub>3</sub> Si[136], B <sub>4</sub> La[137], B <sub>4</sub> Lu[138]
<b>129</b>	$\mathbb{Z}_2 \times \mathbb{Z}_4$	HfSb <sub>2</sub> [139]
<b>136</b>	$\mathbb{Z}_4$	Ag <sub>5</sub> CsSe <sub>3</sub> [140], Ag <sub>5</sub> CsTe <sub>3</sub> [141]
<b>139</b>	$\mathbb{Z}_2 \times \mathbb{Z}_8$	Ag <sub>2</sub> Zr[142], BaCd <sub>2</sub> Ge <sub>2</sub> [143], BaGe <sub>2</sub> Mg <sub>2</sub> [144] CaGe <sub>2</sub> Zn <sub>2</sub> [144], Cd <sub>2</sub> Ge <sub>2</sub> Sr[145], Ge <sub>2</sub> SrZn <sub>2</sub> [146], InPd <sub>3</sub> [147], Pd <sub>2</sub> Ti[148]

Part 2 of Table I:

<b>140</b>	$\mathbb{Z}_2 \times \mathbb{Z}_8$	<a href="#">Hf<sub>2</sub>Si[149]</a> , <a href="#">SiZr<sub>2</sub>[150]</a> , <a href="#">Sb<sub>2</sub>Ti[151]</a> , <a href="#">Si<sub>3</sub>Sr<sub>5</sub>[152]</a> , <a href="#">Sn<sub>3</sub>Sr<sub>5</sub>[153]</a>
<b>164</b>	$\mathbb{Z}_2 \times \mathbb{Z}_4$	<a href="#">Ag<sub>2</sub>O[154]</a> , <a href="#">As<sub>2</sub>Ge<sub>5</sub>Te<sub>8</sub>[155]</a> , <a href="#">As<sub>4</sub>GeTe<sub>7</sub>[156]</a> , <a href="#">BaSn<sub>2</sub>[157, 158]</a> , <a href="#">Be[159]</a> , <a href="#">Bi<sub>2</sub>Li<sub>3</sub>Y[160]</a> , <a href="#">Bi<sub>2</sub>Mg<sub>3</sub>[161, 162]</a> , <a href="#">Bi<sub>2</sub>Pb<sub>2</sub>Se<sub>5</sub>[163, 164]</a> , <a href="#">Bi<sub>4</sub>SnTe<sub>7</sub>[165]</a> , <a href="#">CNb<sub>2</sub>[166]</a> , <a href="#">CTa<sub>2</sub>[167]</a> , <a href="#">C<sub>6</sub>K<sub>2</sub>N<sub>6</sub>PtS<sub>6</sub>[168]</a> , <a href="#">C<sub>6</sub>N<sub>6</sub>PtRb<sub>2</sub>S<sub>6</sub>[168]</a> , <a href="#">CaGe<sub>2</sub>[169, 170]</a> , <a href="#">CaSi<sub>2</sub>[170, 171]</a> , <a href="#">GeSb<sub>4</sub>Te<sub>7</sub>[172]</a> , <a href="#">Ge<sub>2</sub>Sr[170, 173]</a> , <a href="#">PdTe<sub>2</sub>[174, 175]</a> , <a href="#">PtTe<sub>2</sub>[176, 177]</a> , <a href="#">Sb<sub>2</sub>Te<sub>2</sub>[178]</a> , <a href="#">SiTe<sub>2</sub>[179]</a>
<b>166</b>	$\mathbb{Z}_2 \times \mathbb{Z}_4$	<a href="#">Cl<sub>8</sub>Na<sub>2</sub>Ti<sub>3</sub>[180]</a> , <a href="#">Al<sub>10</sub>Ba<sub>7</sub>[181]</a> , <a href="#">As[182]</a> , <a href="#">As<sub>2</sub>CaGa<sub>2</sub>[183]</a> , <a href="#">As<sub>2</sub>Ge<sub>4</sub>Te<sub>7</sub>[184]</a> , <a href="#">As<sub>2</sub>Sn<sub>2</sub>Sr[185, 186]</a> , <a href="#">Bi<sub>2</sub>GeTe<sub>4</sub>[187, 188]</a> , <a href="#">Bi<sub>2</sub>PbTe<sub>4</sub>[189]</a> , <a href="#">Bi<sub>2</sub>SeTe<sub>2</sub>[190, 191]</a> , <a href="#">Bi<sub>2</sub>Se<sub>3</sub>[192, 193]</a> , <a href="#">Bi<sub>2</sub>Te<sub>3</sub>[193, 194]</a> , <a href="#">Bi<sub>6</sub>PbTe<sub>10</sub>[194]</a> , <a href="#">CS<sub>2</sub>Ta<sub>2</sub>[195]</a> , <a href="#">CY<sub>2</sub>[196]</a> , <a href="#">C<sub>5</sub>Ti<sub>8</sub>[197]</a> , <a href="#">CaGe<sub>2</sub>[198]</a> , <a href="#">CaSi<sub>2</sub>[199, 200]</a> , <a href="#">GaGeTe[201]</a> , <a href="#">GaP[202]</a> , <a href="#">In<sub>2</sub>Te<sub>3</sub>[203]</a> , <a href="#">N<sub>2</sub>W[204]</a> , <a href="#">Sb[205]</a> , <a href="#">Sb<sub>2</sub>Te<sub>2</sub>Tl[206, 207]</a> , <a href="#">Sb<sub>2</sub>SeTe<sub>2</sub>[208, 209]</a> , <a href="#">Sb<sub>2</sub>SnTe<sub>4</sub>[210, 211]</a> , <a href="#">Sb<sub>2</sub>Te<sub>3</sub>[193, 212]</a> , <a href="#">Sb<sub>8</sub>Te<sub>3</sub>[213]</a> , <a href="#">Sb<sub>48</sub>Te<sub>9</sub>[213]</a> , <a href="#">ClLa[214]</a>
<b>191</b>	$\mathbb{Z}_6 \times \mathbb{Z}_{12}$	<a href="#">B<sub>2</sub>Sr[215]</a> , <a href="#">BaSi<sub>2</sub>[216]</a> , <a href="#">CaSi<sub>2</sub>[217]</a> , <a href="#">Ti[218]</a>
<b>193</b>	$\mathbb{Z}_{12}$	<a href="#">Pb<sub>3</sub>TeZr<sub>5</sub>[219]</a>
<b>194</b>	$\mathbb{Z}_{12}$	<a href="#">AlN<sub>3</sub>Ti<sub>4</sub>[220]</a> , <a href="#">Al<sub>2</sub>Hf[221]</a> , <a href="#">C<sub>2</sub>AlTa<sub>3</sub>[222]</a> , <a href="#">Ca<sub>2</sub>IN[223]</a> , <a href="#">MgPo[224]</a> , <a href="#">SiSr<sub>2</sub>[225]</a>
<b>216</b>	$\mathbb{Z}_2$	<a href="#">AgKO[226]</a> , <a href="#">AgNaO[226]</a> , <a href="#">AgORB[226]</a> , <a href="#">HgS[227]</a> , <a href="#">InN[228]</a> , <a href="#">NTl[229]</a>
<b>221</b>	$\mathbb{Z}_4 \times \mathbb{Z}_8$	<a href="#">AlSc[230]</a> , <a href="#">AlY[231]</a> , <a href="#">B<sub>6</sub>Ca[232]</a> , <a href="#">B<sub>6</sub>Sr[232]</a> , <a href="#">BeTi[233]</a> , <a href="#">Br<sub>3</sub>CsGe[234]</a> , <a href="#">Br<sub>3</sub>CsPb[235]</a> , <a href="#">CsI<sub>3</sub>Sn[236]</a> , <a href="#">PbSe[237]</a>
<b>223</b>	$\mathbb{Z}_4$	<a href="#">BiNb<sub>3</sub>[238]</a> , <a href="#">Nb<sub>3</sub>Sb[239]</a> , <a href="#">SbTa<sub>3</sub>[240, 241]</a>
<b>225</b>	$\mathbb{Z}_8$	<a href="#">BiY[242]</a> , <a href="#">CZr[243]</a> , <a href="#">Li<sub>2</sub>MgSi[244]</a> , <a href="#">N<sub>2</sub>Pd[245]</a> , <a href="#">AsLa[246, 247]</a> , <a href="#">BiLa[246, 247]</a> , <a href="#">BiLu[248]</a> , <a href="#">LaP[247, 249]</a> , <a href="#">LaSb[247, 250]</a>
<b>227</b>	$\mathbb{Z}_4$	<a href="#">CTi<sub>2</sub>[251]</a> , <a href="#">Se[252]</a>

We list all the relatively good topological crystalline insulators found in our database topological materials searches by GGA calculations in the following table. We give all the structure references behind the names of these materials. Through a further checking by the MBJ calculations, if the GGA calculations predicted band topology is maintained, we print the material name in blue. While in some cases, the MBJ calculations, however, predict a TI phase, we print the name in red. For the materials whose names are in black, the MBJ calculations mostly predict a trivial insulator though they are predicted as TCIs by GGA calculations. In very few cases, the MBJ calculations predict a (semi-)metal phase.

$\mathcal{SG}$	$X_{BS}$	Topological crystalline insulators
<b>2</b>	$\mathbb{Z}_2^3 \times \mathbb{Z}_4$	CsHg[253]
<b>11</b>	$\mathbb{Z}_2^2 \times \mathbb{Z}_4$	BaSb[254], MoTe <sub>2</sub> [255], Sb <sub>2</sub> Sr[256], Se <sub>3</sub> Ta[257, 258]
<b>12</b>	$\mathbb{Z}_2^2 \times \mathbb{Z}_4$	Al <sub>4</sub> Cl <sub>51</sub> Zr <sub>12</sub> [259], Al <sub>4</sub> Na <sub>4</sub> P <sub>12</sub> Sr <sub>8</sub> [260], As <sub>2</sub> Nb[261, 262], As <sub>2</sub> Ta[262, 263], As <sub>3</sub> Mo <sub>2</sub> [264], As <sub>3</sub> W <sub>2</sub> [265] As <sub>4</sub> Ba <sub>3</sub> Zn <sub>2</sub> [266], Ba <sub>3</sub> Cd <sub>2</sub> Sb <sub>4</sub> [267], BiBr[268], BiHf <sub>2</sub> [269], Bi <sub>2</sub> ITe[270, 271], CdK <sub>6</sub> Pb <sub>8</sub> [272], ClZr [273] Cl <sub>8</sub> NSc <sub>5</sub> [274], NbP <sub>2</sub> [275], NbSb <sub>2</sub> [276], Sb <sub>2</sub> Ta[277, 278], Se <sub>4</sub> Ti <sub>3</sub> [279], Ta <sub>2</sub> Te <sub>3</sub> [280], Ge <sub>2</sub> Re[281]
<b>14</b>	$\mathbb{Z}_2 \times \mathbb{Z}_4$	LaSbSe[282], AsSY[283], LaSbSe[282]
<b>51</b>	$\mathbb{Z}_2^2 \times \mathbb{Z}_4$	GaPt <sub>2</sub> [284]
<b>55</b>	$\mathbb{Z}_2 \times \mathbb{Z}_4$	Ca <sub>5</sub> Ga <sub>2</sub> Sb <sub>6</sub> [285]
<b>58</b>	$\mathbb{Z}_4$	Bi <sub>3</sub> RbS <sub>5</sub> [286]
<b>59</b>	$\mathbb{Z}_2 \times \mathbb{Z}_4$	BrNTi[287]
<b>62</b>	$\mathbb{Z}_4$	HgSr <sub>3</sub> [288], LaSbTe[289]
<b>63</b>	$\mathbb{Z}_2 \times \mathbb{Z}_4$	BaGe[290], BaSi[291], BaSn[292], BaPb[293], Ba <sub>3</sub> Pb <sub>5</sub> [294], Ca <sub>2</sub> InN[295], Ba <sub>5</sub> Cd <sub>2</sub> FSb <sub>5</sub> [296], CaGe[297], CaSn Cd <sub>2</sub> FSb <sub>5</sub> Sr <sub>5</sub> [299], PbSr[300], SnSr[301], AlGeLu[302], La <sub>2</sub> Li <sub>2</sub> Si <sub>3</sub> [303], Ge <sub>3</sub> La <sub>2</sub> Li <sub>2</sub> [304]
<b>64</b>	$\mathbb{Z}_2 \times \mathbb{Z}_4$	Ca <sub>5</sub> Ga <sub>2</sub> N <sub>4</sub> [305], Li[306]
<b>69</b>	$\mathbb{Z}_2^2 \times \mathbb{Z}_4$	Ge <sub>6</sub> Li <sub>2</sub> Sr <sub>4</sub> [307]
<b>71</b>	$\mathbb{Z}_2 \times \mathbb{Z}_4$	Ba <sub>3</sub> Bi <sub>4</sub> Li <sub>4</sub> [308], Ba <sub>3</sub> Li <sub>4</sub> Sb <sub>4</sub> [308]
<b>87</b>	$\mathbb{Z}_2 \times \mathbb{Z}_8$	Au <sub>4</sub> Ti[309]
<b>88</b>	$\mathbb{Z}_4$	O <sub>4</sub> PbPd <sub>2</sub> [310]
<b>123</b>	$\mathbb{Z}_2 \times \mathbb{Z}_4 \times \mathbb{Z}_8$	As <sub>3</sub> CsZn <sub>4</sub> [311], As <sub>3</sub> RbZn <sub>4</sub> [311], Pd <sub>3</sub> Sn[312]
<b>129</b>	$\mathbb{Z}_2 \times \mathbb{Z}_4$	AsGeNb[313], GeHfS[314, 315], GeHfSe[314, 315], GeHfTe[314, 315], GeNbSb[316], GeSZr [317] GeSeZr[314], HfSSi[314, 315], HfSeSi[314, 315], OSiZr[314], SSiZr[318], SeSiZr[318], SiTeZr[318], SnTeZr[318]
<b>137</b>	$\mathbb{Z}_4$	Ba <sub>2</sub> LiN[319]
<b>139</b>	$\mathbb{Z}_2 \times \mathbb{Z}_8$	AsBa <sub>2</sub> [320], AsCa <sub>2</sub> [321] Ba <sub>2</sub> Bi[322], Ba <sub>2</sub> Sb[323], BiSr <sub>2</sub> [323], Bi <sub>2</sub> F <sub>2</sub> OSr <sub>2</sub> Ti <sub>2</sub> [324], Br <sub>2</sub> Ca <sub>3</sub> Si [325], SbSr <sub>2</sub> [326]
<b>140</b>	$\mathbb{Z}_2 \times \mathbb{Z}_8$	Bi[327], GePt <sub>3</sub> [328]
<b>148</b>	$\mathbb{Z}_2 \times \mathbb{Z}_4$	Mo <sub>3</sub> S <sub>4</sub> [329]
<b>164</b>	$\mathbb{Z}_2 \times \mathbb{Z}_4$	BaSi <sub>2</sub> [330], BiTe[331], Bi <sub>2</sub> Pb <sub>2</sub> Te <sub>5</sub> [332, 333], Bi <sub>2</sub> Se <sub>2</sub> [334], Bi <sub>3</sub> STe <sub>2</sub> [335], Te <sub>2</sub> Zr[336]
<b>166</b>	$\mathbb{Z}_2 \times \mathbb{Z}_4$	AsNaTe <sub>2</sub> Zr <sub>2</sub> [337], As <sub>3</sub> Cd <sub>4</sub> K[338] As <sub>3</sub> Cd <sub>4</sub> Na[338], As <sub>3</sub> Cd <sub>4</sub> Rb[338], Bi[339], Bi <sub>4</sub> Se <sub>3</sub> [340, 341], Bi <sub>8</sub> Se <sub>9</sub> [342], BrZr[343], CNb <sub>2</sub> S <sub>2</sub> [344] ClZr[273], Hg[345], P[346] BrLa[347]
<b>187</b>	$\mathbb{Z}_3 \times \mathbb{Z}_3$	CHf[348], InNbSe <sub>2</sub> [349, 350], NY[351]
<b>189</b>	$\mathbb{Z}_3 \times \mathbb{Z}_3$	AgAsCa[4, 352], AgCaP[4, 353] GeLiY[354], AsLuPd[355]
<b>191</b>	$\mathbb{Z}_6 \times \mathbb{Z}_{12}$	B <sub>2</sub> Zr[356]
<b>193</b>	$\mathbb{Z}_{12}$	Pb <sub>3</sub> SZr <sub>5</sub> [357]
<b>194</b>	$\mathbb{Z}_{12}$	AsHgK[358, 359], C[360], CdNa <sub>2</sub> Sn[361], HgKSB[359, 362], SnTi <sub>2</sub> [363]
<b>221</b>	$\mathbb{Z}_4 \times \mathbb{Z}_8$	Ba <sub>3</sub> OPb[364, 365], CaPd[366], Ca <sub>3</sub> GeO[364, 365], Ca <sub>3</sub> OPb[365, 367], Ca <sub>3</sub> OSn[364], NTi <sub>3</sub> Tl[368] NY[369], OPbSr <sub>3</sub> [364, 365], PbPt <sub>3</sub> [370], Pt <sub>3</sub> Sn[371]
<b>225</b>	$\mathbb{Z}_8$	AsSc[372], Au <sub>2</sub> InSc[373], Au <sub>2</sub> InY[374], Ba[375], BiI <sub>3</sub> [376], BiSc[377] CPt[378], Ca[205], SSn[379], SbSc[380], SeSn[381], SnTe[382, 383], LuSb[384]
<b>227</b>	$\mathbb{Z}_4$	S <sub>2</sub> Ti[385]

TABLE II. The list of 142 TCIs with clean Fermi surfaces discovered by GGA calculations where the color blue denotes that the MBJ calculation doesn't change the band topology while the red color means that the MBJ calculation results in a strong insulator. Note that the elements in a compound are arranged in the alphabetical order, e.g., TiS<sub>2</sub> is listed as S<sub>2</sub>Ti.

We further highlight a few exceptionally promising candidates which have a full band gap larger than or equal to room temperature, i.e.,  $\geq 25$  meV. They are listed in Table III. Importantly, this list of materials demonstrates a large chemical and structural diversity, which will hopefully provide new topological materials classes that do not suffer from the practical limitations of growing high-quality, insulating samples of the famous  $\text{Bi}_2\text{Se}_3$  family for strong TI materials [386–388] and the SnTe family for TCIs [389, 390].

In addition to the TIs and TCIs highlighted in Table III, there are also many TIs/TCIs with sizable direct band gap and small Fermi pockets in Tables I and II. Despite lacking full band gaps, they nonetheless have relatively large direct continuous gaps throughout the Brillouin zone (BZ). Therefore, these TIs/TCIs might also display robust topological features, and depending on the elements involved they could be favorable for certain specific applications. We believe these compounds also deserve future research attention.

Material name (space group)	Prediction (Method)	Full band gap
$\text{Sb}_2\text{Sr}$ ( <i>SG11</i> )	TI (MBJ)	120 meV
$\text{Al}_2\text{Ge}_4\text{Sr}_3$ ( <i>SG12</i> )	TI (MBJ)	26 meV
$\text{Ba}_{11}\text{Bi}_{14}\text{Cd}_8$ ( <i>SG12</i> )	TI (MBJ)	34 meV
$\text{O}_2\text{Pb}$ ( <i>SG60</i> )	TI (GGA)	40 meV
$\text{AsCdNa}$ ( <i>SG62</i> )	TI (GGA)	87 meV
$\text{Br}_2\text{Ca}_3\text{Si}$ ( <i>SG71</i> )	TI (GGA)	50 meV
$\text{Ag}_5\text{CsSe}_3$ ( <i>SG136</i> )	TI (GGA)	40 meV
$\text{Ag}_5\text{CsTe}_3$ ( <i>SG136</i> )	TI (GGA)	46 meV
$\text{C}_6\text{K}_2\text{N}_6\text{PtS}_6$ ( <i>SG164</i> )	TI (GGA)	50 meV
$\text{C}_6\text{N}_6\text{Rb}_2\text{PtS}_6$ ( <i>SG164</i> )	TI (GGA)	55 meV
$\text{As}_2\text{Sn}_2\text{Sr}$ ( <i>SG166</i> )	TI (GGA)	30 meV
$\text{GaGeTe}$ ( <i>SG166</i> )	TI (GGA)	25 meV
$\text{HgS}$ ( <i>SG216</i> )	TI (GGA)	150 meV
$\text{Bi}_2\text{Pb}_2\text{Te}_5$ ( <i>SG164</i> )	TCI (MBJ)	40 meV
$\text{Bi}_2\text{Se}_2$ ( <i>SG164</i> )	TCI (MBJ)	25 meV

TABLE III. Good TI or TCI candidates with band gap larger than or equal to 25 meV. We give both the topological predictions together with the method used (GGA or MBJ) and the corresponding full band gaps. For comparison, the band gap for the strong TI  $\text{Bi}_2\text{Se}_3$  is 258 meV (GGA) and that for the TCI SnTe is 234 meV (GGA). Note that the elements in a compound are arranged in the alphabetical order, e.g.,  $\text{Sr}_3(\text{AlGe}_2)_2$  is listed as  $\text{Al}_2\text{Ge}_4\text{Sr}_3$ .

### III. TOPOLOGICAL (SEMI-)METALS

We list all the relatively good topological (semi-)metals found in our database topological materials search by GGA calculations in the following table. Each material belongs to a specialized  $\mathcal{SG}$ , and we give all the structure references behind each the name.

Part 1 of Table IV:

TABLE IV. The list of 692 topological (semi-)metals with relatively clean Fermi surfaces discovered based on the GGA calculations: Note that the elements in a compound are arranged in the alphabetical order, e.g., Cd<sub>3</sub>As<sub>2</sub> is listed as As<sub>2</sub>Cd<sub>3</sub>.

<i>Sg</i>	Topological (semi-)metals
11	Br <sub>9</sub> TeW[391],CBrHgNS[392],Li <sub>7</sub> Sn <sub>3</sub> [393],Mo <sub>2</sub> S <sub>2</sub> Sb[394]
15	BaI <sub>4</sub> La[395]
51	AuCd[396],AuTi[397]
52	Ag <sub>2</sub> BiO <sub>3</sub> [398],Bi <sub>3</sub> Sr <sub>2</sub> [399]
55	Al <sub>3</sub> Pd <sub>5</sub> [400],Al <sub>3</sub> Pt <sub>5</sub> [401],BCl <sub>6</sub> Sc <sub>4</sub> [402], Bi <sub>9</sub> Ca <sub>9</sub> Cd <sub>4</sub> [403], Bi <sub>9</sub> Ca <sub>9</sub> Zn <sub>4</sub> [404],Bi <sub>9</sub> Cd <sub>4</sub> Sr <sub>9</sub> [403],In <sub>5</sub> S <sub>13</sub> Y <sub>4</sub> [405]
57	AlCaPd[406], BiK <sub>2</sub> Sn[407]
58	C <sub>60</sub> K[408]
59	Ag <sub>3</sub> Sn[409]
60	F <sub>4</sub> NaTi[410],O <sub>2</sub> Re[411]
61	AgF <sub>2</sub> [412]
	AgAuF <sub>7</sub> [413],AgF <sub>3</sub> K[414],AlPt <sub>2</sub> [415]
	Bi <sub>3</sub> Ca <sub>5</sub> [416],Bi <sub>3</sub> Sr <sub>5</sub> [417],Ca <sub>5</sub> Sb <sub>3</sub> [418]
62	GeNb <sub>3</sub> Te <sub>6</sub> [419],GePd <sub>2</sub> Y[420],N <sub>3</sub> Nb <sub>2</sub> [421],Nb <sub>3</sub> Si[422] PdSbZr[423],SiTa <sub>3</sub> Te <sub>6</sub> [423],AuLu <sub>2</sub> [424],GeLa[425],GeLaPd <sub>2</sub> [425],GeLuPd <sub>2</sub> [426],LuPd <sub>2</sub> Si[427],LuPt[428],LuPt <sub>2</sub> Si[429]
63	AgCa[430], AuCa[431], BiZr[432], Ga <sub>3</sub> PdSr[433], Ga <sub>5</sub> Zr <sub>3</sub> [434], GeSc[435], GeY[436], HfSb[437],K <sub>3</sub> O <sub>4</sub> Pd <sub>2</sub> [438],K <sub>3</sub> O <sub>4</sub> Pt <sub>2</sub> [439],K <sub>4</sub> P <sub>3</sub> [440], N <sub>5</sub> NaTa <sub>3</sub> [442],PdY[443],SiY[444], Sr <sub>3</sub> Tl <sub>5</sub> [445],LuSi[446],Al <sub>6</sub> Re[447]
64	AgCs <sub>2</sub> F <sub>4</sub> [448],Au <sub>10</sub> Ca <sub>4</sub> In <sub>3</sub> [449],Bi[450, 451],LaSb <sub>2</sub> [452]
65	C <sub>7</sub> Re <sub>2</sub> Sc <sub>5</sub> [453],Ge <sub>10</sub> La <sub>7</sub> Li <sub>8</sub> [454]
71	ReSi <sub>2</sub> [455]
74	Ag <sub>2</sub> La[456],Au <sub>2</sub> La[456],In <sub>2</sub> La[457]
87	Ba <sub>9</sub> In <sub>4</sub> [458],In <sub>4</sub> Pd <sub>17</sub> Se <sub>4</sub> [459],Pt <sub>11</sub> Zr <sub>9</sub> [460], Pt <sub>12</sub> Si <sub>5</sub> [461]
88	Al <sub>21</sub> Pt <sub>8</sub> [462],CsFO <sub>3</sub> S[463],Ge <sub>8</sub> Pd <sub>21</sub> [464],LaO <sub>4</sub> Pd <sub>2</sub> [465]
123	AgPPt <sub>5</sub> [466],AlPPt <sub>5</sub> [466],AsInPd <sub>5</sub> [467],AsPd <sub>5</sub> Tl[468] AsPt <sub>5</sub> Tl[468],As <sub>2</sub> BaPd <sub>2</sub> [469],BaP <sub>2</sub> Pd <sub>2</sub> [470],CaPb[471] CdPd[472],CdPd <sub>5</sub> Se[473],CdPt[474],Cd <sub>3</sub> Zr[475] FKNb <sub>4</sub> O <sub>5</sub> [476],HgPd[477],HgPd <sub>5</sub> Se[478],HgPt[479],Hg <sub>2</sub> Pt[479] InPPd <sub>5</sub> [480],InPPt <sub>5</sub> [480],PPd <sub>5</sub> Tl[480],PPt <sub>5</sub> Tl[480] PdTl[481],Pd <sub>5</sub> SeZn[482],SiSr[483],Sr[484],C <sub>2</sub> Re[485],AsLa[486],LaSb[487]
127	AlSc <sub>2</sub> Si <sub>2</sub> [488],Au <sub>2</sub> Ca <sub>2</sub> Pb[489],Au <sub>2</sub> In <sub>2</sub> Y <sub>2</sub> [490],B <sub>2</sub> Ta <sub>3</sub> [491] B <sub>4</sub> W[492],C <sub>2</sub> B <sub>2</sub> Y[493],Ga <sub>2</sub> MgSc <sub>2</sub> [494],Ca <sub>3</sub> Hg <sub>2</sub> [495] Ga <sub>2</sub> Nb <sub>3</sub> [496],Ga <sub>2</sub> Ta <sub>3</sub> [497],Ge <sub>2</sub> Hf <sub>3</sub> [498],Hg <sub>2</sub> Sr <sub>3</sub> [499, 500] InPd <sub>2</sub> Y <sub>2</sub> [501],In <sub>5</sub> Ti <sub>2</sub> [502],LiSi <sub>2</sub> Y <sub>2</sub> [503],PbPd <sub>2</sub> Y <sub>2</sub> [504],N <sub>2</sub> Re[505]
129	AgMgSb[506],AsNbSi[507],AsSiTa[508], BaMgSi[509],BiKMg[510],GeTeZr[511],MoNTa[512]
130	AlMg <sub>4</sub> Si <sub>3</sub> [513],Se <sub>3</sub> Tl <sub>5</sub> [514]
131	OPd[515]
136	AlNb <sub>2</sub> [516],AlTa <sub>2</sub> [517],Bi <sub>2</sub> MgO <sub>6</sub> [518], O <sub>2</sub> Pb[519, 520],O <sub>2</sub> Pd[521],O <sub>2</sub> Pt[522],O <sub>2</sub> Re[523]
137	As <sub>2</sub> Cd <sub>3</sub> [524, 525],Bi <sub>2</sub> Se <sub>3</sub> [526]
139	Ag <sub>2</sub> CaGe <sub>2</sub> [527],Ag <sub>2</sub> Ge <sub>2</sub> Sr[527],Ag <sub>2</sub> Si <sub>2</sub> Sr[528],Ag <sub>2</sub> Sn <sub>2</sub> Sr[529],Al <sub>2</sub> BaSi <sub>2</sub> [530],Al <sub>2</sub> Pb <sub>2</sub> Sr[531],Al <sub>3</sub> Nb[532] Al <sub>3</sub> Ta[533],Al <sub>3</sub> Zr[534],Al <sub>4</sub> Ba[535],Au <sub>4</sub> CaCd <sub>2</sub> [536],BaBi <sub>4</sub> Cl <sub>2</sub> O <sub>6</sub> [537],BaIn <sub>4</sub> [538],Be <sub>12</sub> Pd[539],Be <sub>12</sub> Pt[539] CaGa <sub>4</sub> [540],Ca <sub>11</sub> Sb <sub>10</sub> [541],Ga <sub>3</sub> Nb[542, 543],Ga <sub>3</sub> Ta[544],In <sub>4</sub> Sr[545],Pt <sub>3</sub> Sb[546],S <sub>2</sub> Ti[547],Sb <sub>10</sub> Sr <sub>11</sub> [548] Si <sub>2</sub> W[549],ZnZr <sub>2</sub> [550],Ag <sub>2</sub> Lu[551],Au <sub>2</sub> Lu[552]
140	AgCsF <sub>3</sub> [553],AgF <sub>3</sub> Rb[553],AgIn <sub>2</sub> [554],AlZr <sub>2</sub> [555],AuSe <sub>3</sub> Tl <sub>4</sub> [556],AuTl <sub>2</sub> [557],Au <sub>3</sub> Cd <sub>5</sub> [558] Au <sub>4</sub> In <sub>2</sub> K[559],Au <sub>4</sub> In <sub>2</sub> Rb[559] BGe <sub>2</sub> Nb <sub>5</sub> [560],BMo <sub>2</sub> [561],BTa <sub>2</sub> [562],BTi <sub>2</sub> [563],BW <sub>2</sub> [564],Ba[565],BeTa <sub>2</sub> [566],Bi <sub>3</sub> In <sub>4</sub> Pb[567] Ca <sub>5</sub> Pt <sub>3</sub> [568],Ca <sub>5</sub> Si <sub>3</sub> [569] Cs <sub>9</sub> InO <sub>4</sub> [570],GaHf <sub>2</sub> [571],GaPt <sub>3</sub> [572],GaZr <sub>2</sub> [573],Ga <sub>5</sub> Pd[574],GeHf <sub>2</sub> [575],Ge <sub>3</sub> Mo <sub>5</sub> [576] Ge <sub>3</sub> Nb <sub>5</sub> [577],Ge <sub>3</sub> W <sub>5</sub> [578],Nb <sub>5</sub> SiSn <sub>2</sub> [579] Nb <sub>5</sub> Si <sub>3</sub> [580],Pb <sub>3</sub> Sr <sub>5</sub> [581],PdTl <sub>2</sub> [582],SZr <sub>2</sub> [583] Si <sub>3</sub> W <sub>5</sub> [584],Sr[585],Te <sub>3</sub> Tl <sub>5</sub> [586]
163	AlF <sub>6</sub> LiPd[587],F <sub>6</sub> GaLiPd[588],In <sub>2</sub> Pt <sub>3</sub> [589]
164	AlCl <sub>3</sub> [590],CS <sub>2</sub> [591],CaHg <sub>2</sub> [592],CaSb <sub>2</sub> Zn <sub>2</sub> [593],Cl <sub>2</sub> Ti[594],HfTe <sub>2</sub> [595, 596],Hg <sub>7</sub> K <sub>2</sub> [597] Hg <sub>7</sub> Rb <sub>2</sub> [597],OTi <sub>2</sub> [598],Sb <sub>2</sub> SrZn <sub>2</sub> [599],Se <sub>2</sub> Ti [600]
166	BaPb <sub>3</sub> [601],Be <sub>17</sub> Hf <sub>2</sub> [602],Be <sub>17</sub> Nb <sub>2</sub> [603],Be <sub>17</sub> Ta <sub>2</sub> [602],GeTe[604, 605],Pb <sub>2</sub> Pd <sub>3</sub> S <sub>2</sub> [606] Pb <sub>2</sub> Pd <sub>3</sub> Se <sub>2</sub> [607],Po[608],SbSn [609] AgInSe <sub>2</sub> [610],As <sub>3</sub> NaZn <sub>4</sub> [611],Bi <sub>4</sub> Te <sub>3</sub> [612],C <sub>3</sub> Al <sub>8</sub> N <sub>4</sub> [613],Cd <sub>4</sub> KP <sub>3</sub> [614],GeP <sub>3</sub> [615],In <sub>2</sub> Se <sub>3</sub> [616],Pd <sub>3</sub> Se <sub>2</sub> Tl <sub>2</sub> [617],Ag <sub>4</sub> Sb <sub>2</sub> Sr[618]
167	Al <sub>5</sub> Mo[619],Cs <sub>8</sub> Ga <sub>11</sub> [620],F <sub>3</sub> Mo[621],F <sub>3</sub> Pd[622],F <sub>3</sub> Ti[623],In <sub>11</sub> K <sub>8</sub> [624] K <sub>8</sub> Tl <sub>11</sub> [625],Mo <sub>9</sub> S <sub>11</sub> Tl <sub>2</sub> [626],NPd <sub>3</sub> [627]

Part 2 of Table IV:

	AgCd <sub>3</sub> F <sub>20</sub> Hf <sub>3</sub> [628], AgCd <sub>3</sub> F <sub>20</sub> Zr <sub>3</sub> [628], AgMo <sub>3</sub> Se <sub>3</sub> [629], AsNb <sub>3</sub> Te <sub>3</sub> [630] CsMo <sub>3</sub> S <sub>3</sub> [631], CsMo <sub>3</sub> Se <sub>3</sub> [632], CsMo <sub>3</sub> Te <sub>3</sub> [633], InMo <sub>3</sub> Se <sub>3</sub> [186, 634] InMo <sub>3</sub> Te <sub>3</sub> [186, 634], KM <sub>o</sub> <sub>3</sub> S <sub>3</sub> [634], KM <sub>o</sub> <sub>3</sub> Se <sub>3</sub> [186, 634], KM <sub>o</sub> <sub>3</sub> Te <sub>3</sub> [186, 635], LiMo <sub>3</sub> Se <sub>3</sub> [634] Mo <sub>3</sub> NaSe <sub>3</sub> [186, 634], Mo <sub>3</sub> NaTe <sub>3</sub> [186, 634], Mo <sub>3</sub> RbS <sub>3</sub> [634], Mo <sub>3</sub> RbSe <sub>3</sub> [634, 636] Mo <sub>3</sub> RbTe <sub>3</sub> [637], Mo <sub>3</sub> Se <sub>3</sub> Tl[186, 634], Mo <sub>6</sub> Se <sub>6</sub> Tl <sub>2</sub> [638], NbSe <sub>2</sub> [639]
176	HgPbSr[640], HgSnSr[640], CaHgSn[640], CaHgSn[640]
186	AgN[641], CLiNaO <sub>3</sub> [642], CMo[643], CPt[644], CTa[644], CW[645] InS <sub>2</sub> Ta[646], InSe <sub>2</sub> Ta[647], MoP[648], NNb[649], NPd[650], NW[651] NZr[652], N <sub>2</sub> Pt[653], N <sub>2</sub> Ta[653], NbS[654], STa[655] STi[656], TeZr[657]
187	I <sub>3</sub> LiSc[658]
188	AlHfPt[659], AlPdY[660], AlPtZr[659], Al <sub>2</sub> Hf <sub>6</sub> Pt[661], AsPd <sub>2</sub> [139] AuInY[662], GaPtZr[659], GePdSc[663], GePd <sub>2</sub> [664], GePt <sub>2</sub> [665], InPdY[666] InPtSc[667], InPtY[668], MgPdY[669], NTa[670], PdTlY[671], PdYZn[672] Pd <sub>2</sub> Si[673], PtSb <sub>2</sub> Zr <sub>6</sub> [674], Pt <sub>2</sub> Si[675]
189	AlHfPt[676], AlPtZr[677], B <sub>4</sub> Ga <sub>3</sub> Pt <sub>9</sub> [678], GaHfPd[679], GaPtZr[680], Li <sub>2</sub> Sb[681], PdScSn[682]
190	Au <sub>2</sub> Ba[683], Au <sub>5</sub> K[684], Au <sub>5</sub> Rb[684], B <sub>2</sub> Mo[685], BaGa <sub>2</sub> [686], BaPd <sub>5</sub> [687], Be <sub>2</sub> Hf[688] Be <sub>5</sub> Hf[689], Be <sub>5</sub> Zr[690], CaGa <sub>2</sub> [691], CaHg <sub>2</sub> [692], Hf[693], Hf <sub>2</sub> N <sub>3</sub> Ta[694], Hg[695] LiNNa <sub>2</sub> [696], NNa <sub>3</sub> [697], NOTa[698], NTa[699], N <sub>3</sub> TaTi <sub>2</sub> [700], N <sub>3</sub> TaZr <sub>2</sub> [700], N <sub>4</sub> Ta <sub>2</sub> [699], S <sub>2</sub> Ti[701]
191	AgIn <sub>3</sub> Zr <sub>5</sub> [702], AgPb <sub>3</sub> Zr <sub>5</sub> [703], AgSb <sub>3</sub> Zr <sub>5</sub> [704], AlSn <sub>3</sub> Zr <sub>5</sub> [705], Al <sub>3</sub> Hf <sub>5</sub> [706] Al <sub>3</sub> Hf <sub>5</sub> N[707], Al <sub>3</sub> Ta <sub>5</sub> [708], Al <sub>3</sub> Zr <sub>5</sub> [709], Al <sub>4</sub> Zr <sub>5</sub> [710] AsPb <sub>3</sub> Zr <sub>5</sub> [711], AsSb <sub>3</sub> Zr <sub>5</sub> [712], AsSn <sub>3</sub> Zr <sub>5</sub> [713], As <sub>3</sub> Ca <sub>5</sub> [714], As <sub>3</sub> Sr <sub>5</sub> [715] BNb <sub>5</sub> Si <sub>3</sub> [716], BSn <sub>3</sub> Zr <sub>5</sub> [717], Ba <sub>3</sub> N[718], Ba <sub>5</sub> Bi <sub>3</sub> [719] Ba <sub>5</sub> Sb <sub>3</sub> [719], Bi <sub>3</sub> Sr <sub>5</sub> [720], CSb <sub>3</sub> Zr <sub>5</sub> [721], CSn <sub>3</sub> Zr <sub>5</sub> [722], Ca <sub>5</sub> Sb <sub>3</sub> [723], CdPb <sub>3</sub> Zr <sub>5</sub> [724] Cl <sub>3</sub> Ti[725, 726], Cl <sub>3</sub> Zr[726, 727], GaSn <sub>3</sub> Zr <sub>5</sub> [728], Ga <sub>3</sub> Hf <sub>3</sub> Nb <sub>2</sub> [729] Ga <sub>3</sub> Nb <sub>5</sub> [730], Ga <sub>3</sub> Sc <sub>5</sub> [731], Ga <sub>3</sub> Ta <sub>5</sub> [732], Ga <sub>4</sub> Nb <sub>5</sub> [733], Ga <sub>4</sub> Ti <sub>5</sub> [734] Ga <sub>4</sub> Zr <sub>5</sub> [734], GePb <sub>3</sub> Zr <sub>5</sub> [735], Ge <sub>3</sub> Mo <sub>5</sub> [736], Ge <sub>3</sub> Nb <sub>5</sub> [737] Ge <sub>3</sub> Sc <sub>5</sub> [738], Ge <sub>3</sub> Ta <sub>5</sub> [739], Ge <sub>3</sub> Y <sub>5</sub> [740], HfI <sub>3</sub> [741, 742], Hf <sub>5</sub> Sb <sub>3</sub> Zn[743], Hf <sub>5</sub> Si <sub>3</sub> [744] Hf <sub>5</sub> Sn <sub>3</sub> [706], Hf <sub>5</sub> Sn <sub>4</sub> [745], Hg <sub>3</sub> Mg <sub>5</sub> [746], I <sub>3</sub> Nb[747] I <sub>3</sub> Ti[748, 749], I <sub>3</sub> Zr[750], InPb <sub>3</sub> Zr <sub>5</sub> [751], K <sub>3</sub> Nb <sub>8</sub> O <sub>21</sub> [752] Mo <sub>5</sub> Si <sub>3</sub> [753], NSn <sub>3</sub> Zr <sub>5</sub> [754], N <sub>6</sub> Nb <sub>5</sub> [755], N <sub>6</sub> Ta <sub>5</sub> [756] Nb <sub>5</sub> OPt <sub>3</sub> [757], Nb <sub>5</sub> PSi <sub>3</sub> [758], Nb <sub>5</sub> Si <sub>3</sub> [759], PPb <sub>3</sub> Zr <sub>5</sub> [760] PSn <sub>3</sub> Zr <sub>5</sub> [761], P <sub>3</sub> Ti <sub>5</sub> [762], Pb <sub>3</sub> SbZr <sub>5</sub> [763], Pb <sub>3</sub> Sc <sub>5</sub> [764] Pb <sub>3</sub> SeZr <sub>5</sub> [763], Pb <sub>3</sub> SiZr <sub>5</sub> [763], Pb <sub>3</sub> SnZr <sub>5</sub> [763], Pb <sub>3</sub> Y <sub>5</sub> [765] SSb <sub>3</sub> Zr <sub>5</sub> [766], SSn <sub>3</sub> Zr <sub>5</sub> [767], Sb <sub>3</sub> SiZr <sub>5</sub> [768] Sb <sub>3</sub> Sr <sub>5</sub> [769], Sb <sub>4</sub> Zr <sub>5</sub> [768], SeSn <sub>3</sub> Zr <sub>5</sub> [770], SiSn <sub>3</sub> Zr <sub>5</sub> [770] Si <sub>3</sub> Ta <sub>5</sub> [771], Si <sub>3</sub> Y <sub>5</sub> [772], Sn <sub>4</sub> Zr <sub>5</sub> [745]
193	

Part 3 of Table IV:

	Ag[773], AgAsBa[773], AgAsSr[774], AgBaBi[775], AgBiCa[776], AgBiSr[777], AlPtTi[778], AlYZn[779]
	Al <sub>4</sub> Mg <sub>2</sub> Zn <sub>3</sub> [780], Al <sub>5</sub> Ba <sub>4</sub> [781], AsAuBa[782], AsHf[783]
	AsPdSr[784], AsPtSr[785], AsZr[786], AuBaSb[787], AuBiSr[787]
	AuCaP[788], AuBaP[789], AuCaSb[788], AuKTe[790], AuNaTe[790], AuNa <sub>2</sub> Sn <sub>3</sub> [791], AuRbTe[792]
	AuSbSr[793], AuSe[794], AuSn[795], B <sub>4</sub> Mo[796]
	BaCdGe[797], BaGeZn[797], BaHgSn[797], AlTi <sub>3</sub> [798]
	BaPbZn[797], BaPt[799], BaS <sub>3</sub> Ta[800], BaSe <sub>3</sub> Ta[800], BaSiZn[797], BaSn <sub>3</sub> [801], BaTl <sub>2</sub> [802]
	BiNa <sub>3</sub> [803, 804], BiRb <sub>3</sub> [805], Br <sub>3</sub> RbTi[806], Br <sub>9</sub> Nb <sub>2</sub> Rb <sub>3</sub> [807]
194	Ca[776], CaHgPb[797], CaHgSn[776], CaHg <sub>3</sub> [808]
	CaNa <sub>4</sub> Sn <sub>6</sub> [809], CaPbZn[776], CaPt <sub>2</sub> [810], CaSnZn[776], CdN[811], CdS <sub>2</sub> Ta[812], Cl <sub>3</sub> CsSc[813], Cl <sub>3</sub> CsTi[814]
	Cl <sub>3</sub> RbTi[814], CsI <sub>3</sub> Ti[815]
	GaTi <sub>3</sub> [816], GaYZn[817], Ga <sub>5</sub> Ta <sub>6</sub> [818], GeMg <sub>2</sub> [819], Hf <sub>2</sub> PSb[820], Hf <sub>2</sub> S[821], Hg <sub>3</sub> Sr[822], InMg <sub>3</sub> [823]
	InMoS <sub>2</sub> [824], InTi <sub>3</sub> [825]
	KSn <sub>2</sub> [826], LiTl[827], MgNa <sub>2</sub> Pb[828], MgNa <sub>2</sub> Sn[829], Mg <sub>2</sub> Si[830], Mg <sub>2</sub> Sn[831], NNb[832]
	NnPd[832], NPt[833], N <sub>2</sub> Pt[834], N <sub>2</sub> Ta[834], NaTl[835], NbS <sub>2</sub> [836]
	NbSe <sub>2</sub> [836], O <sub>2</sub> [837], PSbTi <sub>2</sub> [838], PSbZr <sub>2</sub> [839], PTi[840], PbSrZn[841], PdTe[842]
	Pd <sub>3</sub> Zr[843], PoSc[844], S <sub>2</sub> Ta[845], SbTi[846], Sc[847], SrTl <sub>2</sub> [848]
	B <sub>2</sub> Re[849], Be2Re[850], C <sub>2</sub> Re[851], N <sub>2</sub> Re[852], Re[853], AsLaPd[854]
205	AsGa[855], AsIn[855]
	AgAlLi <sub>2</sub> [856], AgBiLi <sub>2</sub> [856, 857], AgMgSb[858], AgLi <sub>2</sub> Sb[856, 857], AlBi[859], AsIn[860], AsTl[861], AuBiCa[862]
216	AuBiLi <sub>2</sub> [863], AuInLi <sub>2</sub> [863], AuLiMgSn[864], AuPbY[865], BBi[861, 866], BiLiMg[867], CdLi <sub>2</sub> Pb[868], CdNa <sub>2</sub> Pb[869]
	CdP <sub>0</sub> [870], GaSb[871], GeInLi[872], GeTi <sub>3</sub> [873], HgSe[874], PTi[875], HgTe[876], InSb[860]
	LiMgPdSb[877], LiMgPtSb [877], MoP[878], PoZn[879], CRe[880]
217	Ge <sub>8</sub> Na <sub>6</sub> Pt <sub>5</sub> [881]
218	Al <sub>6</sub> K <sub>8</sub> O <sub>24</sub> Si <sub>6</sub> [882], Al <sub>6</sub> Na <sub>8</sub> O <sub>24</sub> Si <sub>6</sub> [883]
	AgSc[884], AgY[885], Ag <sub>3</sub> In[886], AlNTi <sub>3</sub> [887], AsSc[888], AsY[889], AuSc[884], AuY[890], Au <sub>3</sub> Li[891]
	BPbSc <sub>3</sub> [892], BPd <sub>3</sub> Sc[893], BPd <sub>3</sub> Y[893], BPt <sub>3</sub> Y[893]
	BaCd[894], BaHg[895], CCaPd <sub>3</sub> [896], Cl <sub>n</sub> Y <sub>3</sub> [897], CTIY <sub>3</sub> [898]
221	C <sub>20</sub> [899], Ca[900], CaTe[901], Ca <sub>3</sub> NTi[902], Ca <sub>3</sub> Pb[903], CdSr[904], CsIO <sub>3</sub> [905], HfPd[906]
	Hg <sub>3</sub> Zr[906], InNTi <sub>3</sub> [907], InSc <sub>3</sub> [908], In <sub>3</sub> Y[909], MgSr[910], MoO <sub>3</sub> Sr[911], NNb[912], NSc[913], PY[914], PbPd <sub>3</sub> [915]
	PbTi[916], PdZr[917], Pd <sub>3</sub> Ti[918], Pd <sub>3</sub> Zr[919], PtTi[920], PtZr[921], Pt <sub>3</sub> Ti[922], SbSc[888], SbTl[923], SbY[924]
	Se[925]
223	CaO <sub>4</sub> Pd <sub>3</sub> [926], CdO <sub>4</sub> Pd <sub>3</sub> [927], O <sub>4</sub> Pd <sub>3</sub> Sr[927], Pd <sub>3</sub> S <sub>4</sub> Y[928], PtTi <sub>3</sub> [929]
224	Ag <sub>2</sub> O[930]
	AgAuCl <sub>6</sub> Cs <sub>2</sub> [931], Ag <sub>2</sub> AlSc[932], Ag <sub>2</sub> InSc[932], Ag <sub>2</sub> InY[933], AsIn[934]
	Be <sub>2</sub> Si[935], BiK <sub>3</sub> [936], Br <sub>6</sub> Cs <sub>2</sub> W[937], Br <sub>6</sub> Rb <sub>2</sub> W[937]
	CTi[938], Ca <sub>2</sub> O <sub>6</sub> PdW[939], CdGeLi <sub>2</sub> [940], CdLi <sub>2</sub> Pb[940]
	Cl <sub>6</sub> Cs <sub>2</sub> Mo[941], Cl <sub>6</sub> Cs <sub>2</sub> W[942], Cl <sub>6</sub> K <sub>2</sub> Mo[943], Cl <sub>6</sub> K <sub>2</sub> W[944]
	Cl <sub>6</sub> MoTl <sub>2</sub> [945], Cl <sub>6</sub> Rb <sub>2</sub> W[946], Cl <sub>6</sub> Tl <sub>2</sub> W[947], F <sub>2</sub> Ti[948]
225	F <sub>6</sub> TiZr[949], GaPd <sub>2</sub> Sc[950], GeHgLi <sub>2</sub> [951], GeLi <sub>2</sub> Pd[952]
	GeLi <sub>2</sub> Zn[953], Hf[954], HgPo[955], HgSe[956], HgTe[957], INaO <sub>6</sub> Pb <sub>2</sub> [958]
	InP[959], InPd <sub>2</sub> Y[960], InPt <sub>2</sub> Sc[961], InSb[962], Li <sub>2</sub> MgPb[963], Li <sub>2</sub> SnZn[964]
	Li <sub>3</sub> Tl[965], Mg <sub>2</sub> Pb[966], Mo[967], O <sub>2</sub> Pt[968], OTi[969]
	OZr[970], Pd[971], Pt[972], Ti[973], Zr[974], LaN[975]
	AgBe <sub>2</sub> [976], Ag <sub>2</sub> Na[977], Al <sub>2</sub> Sc[978], As <sub>2</sub> Na[979]
	AuIn <sub>2</sub> Na <sub>3</sub> [980], Au <sub>2</sub> Bi[981], Au <sub>2</sub> Na[982], Au <sub>2</sub> Pb[983], BaPt <sub>2</sub> [984]
	Be <sub>2</sub> Nb[985], Be <sub>2</sub> Ta[986], Bi <sub>2</sub> Cs[987], Bi <sub>2</sub> K[987], Bi <sub>2</sub> Rb[987], CHf <sub>3</sub> Zn <sub>3</sub> [988]
227	CaLi <sub>2</sub> [989], CaPd <sub>2</sub> [990], CaPt <sub>2</sub> [991], CdLi[992]
	CsGe <sub>17</sub> Na <sub>2</sub> [993], CsO <sub>6</sub> W <sub>2</sub> [994], Ge[995], Ge <sub>136</sub> K <sub>24</sub> [996]
	HfMo <sub>2</sub> [997], HfW <sub>2</sub> [998], LiO <sub>4</sub> Ti <sub>2</sub> [999], LiPt <sub>2</sub> [1000], LiZn[1001], Mo <sub>2</sub> Zr[1002]
	NaPt <sub>2</sub> [1003], Na <sub>2</sub> RbSi <sub>17</sub> [1004], Pd <sub>2</sub> Sr[1005], Pt <sub>2</sub> Sr[1005], Pt <sub>2</sub> Y[1006], Sn[1007], W <sub>2</sub> Zr[1008]
229	Ba[291], Ca[1009], Hf[1010], Sr[1011], Ti[1012], Zr[1013]

#### IV. ALL OF THE PREDICTED TOPOLOGICAL MATERIALS

We listed below all the predicted topological materials predicted by SI theory no matter whether they have clean or dirty Fermi surfaces, i.e. all the TIs from **Case 2** in Table V, all the TCIs from **Case 2** in Table VI and all the TSMs from **Case 3** in Table VII, respectively. We further list materials from **Cases 1** and **2**, but potentially with band crossings near the Fermi energy, in Table VIII.

Part 1 of all the predicted TIs:

TABLE V. All the topological insulators: Note that, due to band dispersions these materials might not be insulating in reality.

<i>SG</i>	Topological insulators
<b>2</b>	AgF <sub>6</sub> Pd,, Ag <sub>2</sub> F <sub>5</sub> , As <sub>3</sub> Ca, As <sub>3</sub> Sr, BaMo <sub>6</sub> S <sub>8</sub> , Bi, Br <sub>5</sub> W, C <sub>5</sub> B, CaP <sub>3</sub> , CaMo <sub>6</sub> S <sub>8</sub> , Mo <sub>3</sub> S <sub>4</sub> , Ga <sub>31</sub> Mo <sub>6</sub> , Mo <sub>6</sub> S <sub>8</sub> Sr, O <sub>18</sub> Ti <sub>10</sub> , Re, Cl <sub>14</sub> Mo <sub>4</sub> O <sub>4</sub> Tl <sub>2</sub> , Bi <sub>9</sub> In <sub>6</sub> K <sub>11</sub> , AgO <sub>4</sub> S,
<b>10</b>	Te <sub>4</sub> TiZr,
<b>11</b>	Sn <sub>2</sub> SrZn <sub>2</sub> , Se <sub>3</sub> Ta <sub>2</sub> , AlAu, BBeLi, Au <sub>2</sub> BaSb <sub>2</sub> , CaSb <sub>2</sub> , Cl <sub>7</sub> CsTi <sub>2</sub> , GeHfPd, HfS <sub>3</sub> , MgZn <sub>2</sub> , Nb <sub>2</sub> Se <sub>3</sub> , Mo <sub>2</sub> S <sub>3</sub> , NbPt <sub>3</sub> , Ga <sub>5</sub> Pt, Bi <sub>7</sub> In <sub>3</sub> Pb <sub>4</sub> S <sub>18</sub> ,
<b>12</b>	Al <sub>2</sub> Ge <sub>4</sub> Sr <sub>3</sub> , Ag <sub>4</sub> K <sub>2</sub> Se <sub>3</sub> , Al <sub>8</sub> Mo <sub>3</sub> , As <sub>3</sub> Ba, As <sub>3</sub> Sr, As <sub>4</sub> Nb <sub>7</sub> , Al <sub>2</sub> Ba <sub>5</sub> Ge <sub>7</sub> , BaSb <sub>3</sub> , BaTl <sub>4</sub> , Au <sub>2</sub> P <sub>3</sub> , Ba <sub>2</sub> Cd <sub>2</sub> Sb <sub>3</sub> , Ba <sub>2</sub> Mg <sub>3</sub> Si <sub>4</sub> , Ba <sub>3</sub> Li <sub>4</sub> Sn <sub>8</sub> , Bi <sub>16</sub> I <sub>4</sub> , Bi <sub>2</sub> Pd, Bi <sub>2</sub> Pd <sub>5</sub> , Bi <sub>2</sub> Pd <sub>3</sub> Se <sub>2</sub> , Bi <sub>2</sub> Pd <sub>3</sub> S <sub>2</sub> , Bi <sub>2</sub> Hg <sub>4</sub> S <sub>4</sub> , Ba <sub>2</sub> Hg <sub>3</sub> O <sub>14</sub> Pd <sub>7</sub> , Au <sub>8</sub> GaK <sub>4</sub> ,
<b>13</b>	Bi <sub>2</sub> Pb <sub>3</sub> S <sub>6</sub> , Bi <sub>4</sub> Pb <sub>7</sub> Se <sub>13</sub> , Ba <sub>11</sub> Bi <sub>14</sub> Cd <sub>8</sub> , Br <sub>4</sub> Cs <sub>2</sub> I <sub>2</sub> Pd, CKN, CaGa <sub>4</sub> , Cl <sub>3</sub> Ti, Cl <sub>10</sub> W <sub>2</sub> , Ga <sub>3</sub> Sc <sub>5</sub> , Ga <sub>7</sub> Rb, Hg, Hg <sub>2</sub> Sn <sub>2</sub> Sr, Li <sub>2</sub> Si, Li <sub>8</sub> Pb <sub>3</sub> , Mg <sub>5</sub> Si <sub>6</sub> , Mg <sub>2</sub> Si <sub>10</sub> Sr <sub>11</sub> , Nb <sub>2</sub> PdSe <sub>6</sub> , Nb <sub>2</sub> PdS <sub>6</sub> , Nb <sub>2</sub> Te <sub>3</sub> , Nb <sub>2</sub> PdS <sub>5</sub> , OTi, O <sub>13</sub> Sr <sub>2</sub> Ti <sub>6</sub> , Mg <sub>4</sub> Zn <sub>7</sub> , P <sub>3</sub> Sr, PdSe <sub>6</sub> Ta <sub>2</sub> , Nb <sub>8</sub> PtSe <sub>20</sub> , PtTe, P <sub>4</sub> Ti <sub>7</sub> , Pt <sub>3</sub> Te <sub>4</sub> , Sc <sub>2</sub> Zr, PtSe <sub>7</sub> Ta <sub>2</sub> , Te, Se <sub>4</sub> Ti <sub>11</sub> , Sc <sub>8</sub> Te <sub>3</sub> , Cl <sub>2</sub> La <sub>3</sub> Si <sub>3</sub> ,
<b>14</b>	Cl <sub>3</sub> NbSe, I <sub>6</sub> Nb <sub>2</sub> Te <sub>2</sub> , Br <sub>6</sub> Nb <sub>2</sub> Se <sub>2</sub> , Br <sub>3</sub> NbSe,
<b>15</b>	As <sub>2</sub> Pt <sub>2</sub> Sr, Ag <sub>2</sub> Te, BK <sub>3</sub> S <sub>3</sub> , BeLiN, BaNb <sub>2</sub> O <sub>6</sub> , Ba <sub>3</sub> P <sub>14</sub> , B <sub>2</sub> S <sub>3</sub> , AuI <sub>4</sub> Li, As <sub>2</sub> F <sub>8</sub> O <sub>2</sub> Rb <sub>2</sub> , Bi,
<b>47</b>	Cl <sub>2</sub> Te <sub>3</sub> , O <sub>3</sub> Pb <sub>2</sub> , O <sub>3</sub> S, O <sub>2</sub> Ti, Br <sub>2</sub> O <sub>5</sub> Sb <sub>4</sub> , Cl <sub>2</sub> O <sub>5</sub> Sb <sub>4</sub> , FGaO <sub>3</sub> Te, Cl <sub>4</sub> Hg <sub>4</sub> I <sub>2</sub> S, Rb <sub>2</sub> S <sub>7</sub> Sb <sub>4</sub> , HfO <sub>2</sub> , NOTa, Cl <sub>6</sub> Hg <sub>3</sub> S <sub>2</sub> Zr,
<b>50</b>	C,
<b>51</b>	AuITe <sub>2</sub> , Au <sub>3</sub> Rb <sub>2</sub> Tl, PtTi, AlPt <sub>2</sub> , CB <sub>2</sub> U, La <sub>2</sub> Se <sub>9</sub> U <sub>2</sub> ,
<b>52</b>	Ca <sub>2</sub> GeIn <sub>2</sub> Sr, F <sub>7</sub> KPd <sub>7</sub> Zr,
<b>55</b>	Al <sub>2</sub> Bi <sub>6</sub> Ca <sub>5</sub> , C <sub>2</sub> B <sub>2</sub> Sc, Se <sub>2</sub> Ti <sub>9</sub> , O <sub>8</sub> W <sub>3</sub> , InLa <sub>2</sub> Si <sub>2</sub> , B <sub>4</sub> MoU, B <sub>4</sub> UW, B <sub>6</sub> U <sub>2</sub> W, ReSi <sub>2</sub> Zr, HfReSi <sub>2</sub> , Bi <sub>6</sub> In <sub>2</sub> Sr <sub>5</sub> ,
<b>57</b>	STa <sub>2</sub> ,
<b>58</b>	Ge <sub>6</sub> Li <sub>2</sub> Sr <sub>4</sub> , Ca <sub>2</sub> Ge <sub>3</sub> Li, S <sub>2</sub> Ti, Bi <sub>2</sub> Hf, Cl <sub>16</sub> Ti <sub>7</sub> , In <sub>2</sub> Se, Br <sub>16</sub> Ti <sub>7</sub> , C <sub>3</sub> Al <sub>2</sub> Th <sub>2</sub> , Au <sub>8</sub> Sn <sub>3</sub> Sr <sub>3</sub> , SeTi <sub>2</sub> , SZr <sub>2</sub> , In <sub>2</sub> Te,
<b>59</b>	Ag <sub>3</sub> Sb, Au <sub>3</sub> In, Au <sub>3</sub> In <sub>3</sub> Sr, Au <sub>3</sub> KSn <sub>3</sub> , AuRb <sub>3</sub> Sn <sub>4</sub> , AuPb <sub>4</sub> Rb <sub>3</sub> , Au <sub>3</sub> Lu, AuCs <sub>3</sub> Pb <sub>4</sub> ,
<b>60</b>	CW <sub>2</sub> , O <sub>2</sub> Pb, Au <sub>2</sub> Pb, MgO <sub>3</sub> Si,
<b>61</b>	AuSn <sub>2</sub> , Bi <sub>2</sub> Pt,
<b>62</b>	AsCdNa, AlPdY, AlPtY, As <sub>2</sub> Hf, As <sub>2</sub> Zr, As <sub>2</sub> Hf <sub>3</sub> , Ba <sub>2</sub> Pb, As <sub>3</sub> Sc <sub>5</sub> , Ba <sub>2</sub> Si, As <sub>3</sub> Nb <sub>5</sub> , FSeY, Bi <sub>3</sub> Sc <sub>5</sub> , Bi <sub>3</sub> Y <sub>5</sub> , GaPtY, GaPdSc, GaPtSc, GaPdY, GeHfPt, Ga <sub>2</sub> Pd <sub>5</sub> , PPtSc, P <sub>2</sub> Zr, P <sub>2</sub> Ti,

Part 2 of all the predicted TIs:

	GeMoZr, PdSiZr, PdSiTi, PbSr <sub>2</sub> , PtSiTi, PtSnSr, PtSiZr, GePdZr, Ca, GePtZr, GeZr, CaCdPd, SiZr, Sb <sub>2</sub> SrZn, SiSr, CaCdPt, SiTi, Ge <sub>2</sub> Mo, SrZn, Ge <sub>2</sub> Li <sub>3</sub> Na, Ge <sub>2</sub> W, Ge <sub>2</sub> InLiSr <sub>2</sub> , Ge <sub>3</sub> Pt <sub>2</sub> , CaGePt, CaMgPd, Ge <sub>4</sub> Hf <sub>3</sub> Nb <sub>2</sub> , PdSc <sub>6</sub> Te <sub>2</sub> , Ge <sub>4</sub> Ti <sub>5</sub> , HfNbP, SeTi <sub>2</sub> , CaPbPd, CaPbPt, CaPdSn, HfP <sub>2</sub> , CaPtSn, HfSi, CaPtSi, Ca <sub>2</sub> Hg, HgMg <sub>2</sub> , Hf <sub>3</sub> P <sub>2</sub> , Ca <sub>3</sub> Pd, Ca <sub>3</sub> GeO, Pd <sub>9</sub> Si <sub>2</sub> , Pb <sub>4</sub> Sr <sub>5</sub> , CdGeSr, CdNaSb, CdPtSr, Ca <sub>2</sub> Pt <sub>3</sub> Sn <sub>5</sub> , Ge <sub>6</sub> Sr <sub>7</sub> , Mg <sub>2</sub> Pb, NNa <sub>3</sub> , N <sub>5</sub> Ta <sub>3</sub> , Mo <sub>4</sub> P <sub>3</sub> , NbPZr, Nb <sub>5</sub> P <sub>3</sub> , AuLa, PdTh, AlLaPt, AlLuPt, GaLuPd, GaLaPd, GaLuPt, Se <sub>2</sub> U, LaPPt, STeU, SeTeU, S <sub>3</sub> U <sub>2</sub> , S <sub>3</sub> Th <sub>2</sub> , Se <sub>3</sub> U <sub>2</sub> , Te <sub>3</sub> U <sub>2</sub> , CaSe <sub>5</sub> U <sub>2</sub> , S <sub>5</sub> TiU <sub>2</sub> , PbS <sub>5</sub> U <sub>2</sub> , Se <sub>5</sub> U <sub>3</sub> , PbSe <sub>5</sub> U <sub>2</sub> , Sn <sub>4</sub> Th <sub>5</sub> , La <sub>2</sub> S <sub>5</sub> U, La <sub>2</sub> Se <sub>5</sub> U, Te <sub>5</sub> U <sub>3</sub> , SrZn <sub>5</sub> , Sc <sub>2</sub> Te, PdTe <sub>2</sub> Y <sub>6</sub> , Pt <sub>4</sub> Sr <sub>5</sub> , TeZr <sub>2</sub> , Ba <sub>7</sub> Ge <sub>6</sub> , Pt <sub>3</sub> Sr <sub>7</sub> , GePdTl, AlAuCa, HfPdSi, HfPtSi,
62	AlBMo, Ag <sub>2</sub> Si, AlBW, AlSc, AlY, AgS <sub>3</sub> Ta, As <sub>2</sub> BaPd, AlHf <sub>3</sub> N, AuIn <sub>2</sub> Na, AuClTe <sub>2</sub> , BNb, BTa, BaCd <sub>2</sub> Pt, BaIn, As <sub>3</sub> Nb <sub>4</sub> , BaIn <sub>2</sub> Pt, BePd <sub>3</sub> , BaZn <sub>5</sub> , Ba <sub>3</sub> Ge <sub>5</sub> , B <sub>7</sub> WY <sub>3</sub> , Ba <sub>3</sub> Sn <sub>5</sub> , CB <sub>3</sub> Nb <sub>3</sub> , CaSi, CaZn, Cd <sub>2</sub> PdSr, CaIn <sub>4</sub> Pd, Ca <sub>2</sub> Sn <sub>6</sub> Zn <sub>3</sub> , GaSc, Ga, GaY, GeNa <sub>2</sub> Zn, Ge <sub>2</sub> Hf, HfPd, HfSi <sub>2</sub> , InSb, HfTe <sub>5</sub> , In <sub>4</sub> PdSr, In <sub>4</sub> PbSr <sub>3</sub> , Mg <sub>2</sub> PdSr, In <sub>2</sub> PtSr, In <sub>4</sub> PtSr, PdZr, Pd <sub>3</sub> Ti <sub>2</sub> , Si <sub>2</sub> Zr, SiZr, SnTi <sub>3</sub> , Sn <sub>4</sub> Sr, TiZn <sub>16</sub> , Tl <sub>5</sub> Y <sub>3</sub> , Sn <sub>5</sub> Sr <sub>3</sub> , Mo <sub>9</sub> Se <sub>11</sub> , U, AuLa, GaLu, GaLa, PtTh, Ge <sub>2</sub> U, Sn <sub>2</sub> Th, Ge <sub>2</sub> Th, BNU, AlLa, Te <sub>3</sub> U, LiLuSn <sub>2</sub> , LaLiSn <sub>2</sub> , La <sub>2</sub> SnZn <sub>5</sub> , GaU, In <sub>5</sub> La <sub>3</sub> , Lu <sub>3</sub> Tl <sub>5</sub> , Ge <sub>6</sub> La <sub>2</sub> Zn <sub>3</sub> , O <sub>8</sub> U <sub>3</sub> , Al <sub>2</sub> BaSi <sub>2</sub> , BaPdSb <sub>2</sub> , Te <sub>5</sub> Zr, As <sub>4</sub> Cd <sub>5</sub> Rb <sub>2</sub> , Ge <sub>8</sub> Na <sub>15</sub> PSn,
63	As, AgNO <sub>3</sub> , Ba <sub>2</sub> Bi <sub>4</sub> Cd <sub>3</sub> , Cs, Ga, Ge, K, Rb, Pd <sub>8</sub> Sn <sub>24</sub> , PdSn <sub>3</sub> , LiTl, Sn <sub>3</sub> Ti <sub>2</sub> , C <sub>2</sub> B <sub>2</sub> Mg, Br <sub>16</sub> W <sub>6</sub> , Ba <sub>2</sub> Ca <sub>2</sub> Sn <sub>6</sub> ,
64	Al <sub>2</sub> Ti, Ag <sub>3</sub> Te <sub>2</sub> Tl, CBY, Ga <sub>2</sub> Zr, Ga <sub>2</sub> Sc, HfPd <sub>5</sub> , Li <sub>7</sub> Sn <sub>2</sub> , Br <sub>2</sub> Cd <sub>2</sub> Hg <sub>2</sub> S <sub>2</sub> , Ba <sub>3</sub> Ge <sub>4</sub> , Ge <sub>2</sub> U, Ge <sub>2</sub> Th, LaSn <sub>2</sub> , AlB <sub>4</sub> Lu, Ge <sub>2</sub> PbSr <sub>2</sub> , PZr <sub>2</sub> ,
65	I <sub>3</sub> Th,
66	Be <sub>2</sub> Zn, Si <sub>2</sub> Ti, Cs <sub>2</sub> Pt <sub>3</sub> Se <sub>6</sub> U, Cs <sub>2</sub> Pt <sub>3</sub> S <sub>6</sub> U,
67	NbSn <sub>2</sub> , Si <sub>2</sub> Ti, Sn <sub>2</sub> Zr, SbSnTi, Rb, Sn <sub>2</sub> Ta, P <sub>2</sub> S <sub>7</sub> U, Ge <sub>2</sub> Ti,
71	Al <sub>2</sub> Ba <sub>3</sub> Ge <sub>2</sub> , Al <sub>2</sub> Ba <sub>3</sub> Si <sub>2</sub> , Al <sub>2</sub> Ba <sub>3</sub> Sn <sub>2</sub> , Al <sub>2</sub> Ca <sub>3</sub> Si <sub>2</sub> , Al <sub>2</sub> Si <sub>2</sub> Sr <sub>3</sub> , Ag <sub>3</sub> Ga <sub>8</sub> Y <sub>3</sub> , AsTeTi, Al <sub>2</sub> Ge <sub>2</sub> Sr <sub>3</sub> , Al <sub>2</sub> Sn <sub>2</sub> Sr <sub>3</sub> , CdO <sub>6</sub> Pt <sub>3</sub> , Ca <sub>3</sub> Ga <sub>8</sub> , Mo <sub>3</sub> Ti, MoPt <sub>2</sub> , Ga <sub>9</sub> Pt <sub>2</sub> Y <sub>3</sub> , Pt <sub>2</sub> W, Ge <sub>5</sub> Ti <sub>6</sub> , Hf <sub>27</sub> P <sub>16</sub> , C <sub>3</sub> Si <sub>2</sub> U <sub>3</sub> , Te <sub>2</sub> U, Nb <sub>6</sub> Sn <sub>5</sub> , N <sub>2</sub> Re, Sn, Pd <sub>2</sub> Ti, Br <sub>2</sub> Ca <sub>3</sub> Si,
72	Ga <sub>2</sub> Mg <sub>5</sub> , In <sub>2</sub> Mg <sub>5</sub> , Pb <sub>5</sub> Sc <sub>6</sub> , Br <sub>2</sub> Hg <sub>5</sub> O <sub>4</sub> ,
73	AlAs <sub>2</sub> Li <sub>3</sub> , Bi <sub>3</sub> K <sub>3</sub> Na <sub>2</sub> Sn,
74	Au <sub>2</sub> Ca, Ag <sub>2</sub> Ca, Ge, BaIn <sub>2</sub> , Si, Ba <sub>2</sub> O <sub>7</sub> U <sub>2</sub> ,
82	AsPd <sub>3</sub> , GeTi <sub>3</sub> , Mo <sub>3</sub> P, TeZr <sub>3</sub> , SbZr <sub>3</sub> , GeTa <sub>3</sub> , Te <sub>3</sub> Tl <sub>5</sub> , PW <sub>3</sub> ,
85	Se <sub>2</sub> U,

Part 3 of all the predicted TIs:

<b>86</b>	GeTa <sub>3</sub> , GeNb <sub>3</sub> , Nb <sub>3</sub> Si,
<b>87</b>	Se <sub>4</sub> Ti <sub>5</sub> , As <sub>4</sub> Mo <sub>5</sub> , Te <sub>4</sub> Zr <sub>5</sub> , Hf <sub>5</sub> Te <sub>4</sub> , O <sub>5</sub> Ti <sub>4</sub> , Te <sub>4</sub> Ti <sub>5</sub> ,
<b>88</b>	CaO <sub>4</sub> Se, GeO <sub>4</sub> U, Pd <sub>2</sub> S <sub>4</sub> U, O <sub>24</sub> Re <sub>4</sub> Sr <sub>11</sub> ,
<b>113</b>	GaNb <sub>4</sub> S <sub>8</sub> ,
<b>114</b>	Pd <sub>4</sub> S,
<b>118</b>	B,
<b>121</b>	Ag <sub>2</sub> S <sub>4</sub> SnZn, Mo <sub>3</sub> P, AuPb <sub>3</sub> , AsHgS <sub>3</sub> Tl,
<b>122</b>	As <sub>2</sub> SnZn, AgInSe <sub>2</sub> , As <sub>2</sub> CdGe, As <sub>2</sub> CdSn, CdSb <sub>2</sub> Sn, F <sub>5</sub> U,
<b>123</b>	BiLi, BiNa, ClNa <sub>3</sub> , HgTi, ClNa <sub>2</sub> , MgPt <sub>3</sub> , AgPPd <sub>5</sub> , BaGe <sub>3</sub> Mg <sub>4</sub> , Pd <sub>5</sub> Ti <sub>3</sub> , Hf <sub>5</sub> Pb, As <sub>2</sub> BaOTi <sub>2</sub> , HgZr, MoPt <sub>3</sub> , N <sub>3</sub> Rb,
<b>125</b>	Pb <sub>4</sub> Pt,
<b>127</b>	CdGe <sub>2</sub> Y <sub>2</sub> , Ca <sub>2</sub> Ge <sub>2</sub> Sn, CsI <sub>3</sub> Sn, Hf <sub>3</sub> In <sub>4</sub> , GaPt <sub>3</sub> , AlPt <sub>3</sub> , B <sub>4</sub> Y, Pt <sub>3</sub> Si, B <sub>4</sub> La, B <sub>4</sub> U, B <sub>4</sub> Lu, Si <sub>2</sub> Th <sub>3</sub> , CB <sub>2</sub> Lu, In <sub>4</sub> Ti <sub>3</sub> ,
<b>129</b>	CdTi, Sc, SeTi, HfSb <sub>2</sub> , AgSb <sub>2</sub> Y, BaGeMg, BaMgSn, CaGaN, BaSn <sub>2</sub> Zn <sub>2</sub> , Al <sub>2</sub> Au <sub>2</sub> Sr, Au <sub>2</sub> Sn <sub>2</sub> Sr, Be <sub>2</sub> CaGe <sub>2</sub> , AsPU, OTeU, Bi <sub>2</sub> LaLi, AuLaSb <sub>2</sub> , Ge <sub>2</sub> Pt <sub>2</sub> U, Ge <sub>2</sub> Pt <sub>2</sub> Th, AgLaSb <sub>2</sub> , CaGa <sub>4</sub> ,
<b>130</b>	Ca <sub>5</sub> Ge <sub>3</sub> , Ba <sub>5</sub> Si <sub>3</sub> , Ga <sub>3</sub> Y <sub>5</sub> ,
<b>131</b>	IPdTe, F <sub>6</sub> PbSr, CaO <sub>4</sub> Pt <sub>2</sub> ,
<b>133</b>	PTa <sub>3</sub> ,
<b>135</b>	Cs, CB <sub>2</sub> Lu, CB <sub>2</sub> Sc,
<b>136</b>	Cd <sub>4</sub> Pt <sub>2</sub> Sr, BaCd <sub>4</sub> Pt <sub>2</sub> , Al <sub>2</sub> Y <sub>3</sub> , Li <sub>2</sub> Sr <sub>3</sub> , BaHg <sub>2</sub> Tl <sub>2</sub> , BaHg <sub>2</sub> Tl <sub>2</sub> , Ag <sub>5</sub> CsTe <sub>3</sub> , Ag <sub>5</sub> CsSe <sub>3</sub> , Al <sub>2</sub> Zr <sub>3</sub> ,
<b>137</b>	Ba <sub>2</sub> S <sub>6</sub> U,
<b>139</b>	Ag <sub>2</sub> Zr, Au <sub>2</sub> Be, Au <sub>2</sub> Hf, Bi <sub>2</sub> Pd, CdHg <sub>2</sub> , Hg <sub>2</sub> Mg, CaGe <sub>2</sub> Zn <sub>2</sub> , CaP <sub>2</sub> Pd <sub>2</sub> , Au <sub>2</sub> CaSi <sub>2</sub> , Au <sub>2</sub> Zr, BaGe <sub>2</sub> Mg <sub>2</sub> , Be <sub>12</sub> W, Ge <sub>2</sub> SrZn <sub>2</sub> , Be <sub>12</sub> Mo, BaCd <sub>2</sub> Ge <sub>2</sub> , Cd <sub>2</sub> Hg, Ga <sub>3</sub> Zr, Cd <sub>2</sub> Ge <sub>2</sub> Sr, Pd <sub>2</sub> Zr, PdZr <sub>2</sub> , Hf <sub>2</sub> Pd, Hg <sub>2</sub> In <sub>2</sub> Sr, Pd <sub>2</sub> Ti, P <sub>2</sub> Pd <sub>2</sub> Sr, Au <sub>2</sub> Si <sub>2</sub> Sr, InPd <sub>3</sub> , In <sub>3</sub> Zr, Pt <sub>8</sub> Ti, Bi <sub>10</sub> Ca <sub>11</sub> , C <sub>2</sub> PtU <sub>2</sub> , Al <sub>2</sub> Pd <sub>5</sub> U, GeTeU, LaSbSc, GeSeU, La <sub>2</sub> O <sub>4</sub> Pd, LuSbZr, O <sub>2</sub> TeU <sub>2</sub> , Pt <sub>2</sub> Si <sub>2</sub> U, SeSiU, La <sub>2</sub> Sb, PdTi <sub>2</sub> , Au <sub>2</sub> Ge <sub>2</sub> Sr, Cd <sub>2</sub> Ga <sub>2</sub> Sr, MgPd <sub>3</sub> , BaBi <sub>4</sub> Br <sub>2</sub> O <sub>6</sub> ,
<b>140</b>	Sc, Sb, BeTa <sub>2</sub> , Hf <sub>2</sub> Si, SiZr <sub>2</sub> , Pb <sub>2</sub> Pt, Sb <sub>2</sub> Ti, SiTa <sub>2</sub> , SbTi <sub>3</sub> , B <sub>2</sub> Mo <sub>5</sub> Si, In <sub>5</sub> Sb <sub>3</sub> , Ga <sub>3</sub> Ta <sub>5</sub> , Bi <sub>3</sub> In <sub>5</sub> , Si <sub>3</sub> Sr <sub>5</sub> , Sn <sub>3</sub> Sr <sub>5</sub> , SiU <sub>3</sub> , BaTe <sub>5</sub> U <sub>2</sub> , PtTl <sub>2</sub> , Ge <sub>3</sub> Sr <sub>5</sub> ,
<b>141</b>	AgLi, Si, Sn, PTa, BW, Ga <sub>2</sub> Hf, S <sub>2</sub> Zr <sub>9</sub> , Ag <sub>8</sub> O <sub>4</sub> S <sub>2</sub> Si, PbU, Ga <sub>2</sub> Th, Ge, NbP, GaZr, In <sub>2</sub> Zr, ScSn <sub>2</sub> , Al <sub>2</sub> Ti,
<b>142</b>	Au <sub>3</sub> Zn,

Part 4 of all the predicted TIs:

<b>147</b>	Ge <sub>9</sub> Pd <sub>25</sub> , O <sub>8</sub> U <sub>3</sub> , Au <sub>7</sub> In <sub>3</sub> ,
<b>148</b>	Bi <sub>2</sub> STe <sub>2</sub> , Mo <sub>3</sub> Se <sub>4</sub> , Cl <sub>12</sub> NSc <sub>7</sub> , Bi <sub>14</sub> S <sub>8</sub> Te <sub>13</sub> ,
<b>162</b>	Ag <sub>6</sub> O <sub>2</sub> , Cl <sub>4</sub> Mo,
<b>164</b>	Be, Ag <sub>2</sub> O, CNb <sub>2</sub> , CaGe <sub>2</sub> , CTa <sub>2</sub> , BaSn <sub>2</sub> , CaSi <sub>2</sub> , CNb <sub>2</sub> S <sub>2</sub> , Bi <sub>2</sub> Mg <sub>3</sub> , CS <sub>2</sub> Ta <sub>2</sub> , Bi <sub>2</sub> Li <sub>3</sub> Y, Bi <sub>2</sub> Pb <sub>2</sub> Se <sub>5</sub> , As <sub>4</sub> GeTe <sub>7</sub> , Bi <sub>4</sub> SnTe <sub>7</sub> , As <sub>2</sub> Ge <sub>5</sub> Te <sub>8</sub> , Cl <sub>8</sub> Nb <sub>3</sub> , C <sub>6</sub> N <sub>6</sub> PtRb <sub>2</sub> S <sub>6</sub> , C <sub>6</sub> K <sub>2</sub> N <sub>6</sub> PtS <sub>6</sub> , Bi <sub>8</sub> Se <sub>7</sub> , Ge <sub>2</sub> Sr, PdTe <sub>2</sub> , PtTe <sub>2</sub> , SiTe <sub>2</sub> , GeSb <sub>4</sub> Te <sub>7</sub> , Sb <sub>2</sub> Te <sub>2</sub> , Te <sub>6</sub> Zr <sub>5</sub> , Sb <sub>2</sub> Te,
<b>166</b>	As, CaSi <sub>2</sub> , GaP, CS <sub>2</sub> Ta <sub>2</sub> , In <sub>2</sub> Te <sub>3</sub> , GaGeTe, CY <sub>2</sub> , STi, Bi <sub>2</sub> GeTe <sub>4</sub> , Ga <sub>2</sub> Te <sub>3</sub> , Sb, S <sub>2</sub> Ta, SeTi, As <sub>2</sub> Sn <sub>2</sub> Sr, N <sub>2</sub> W, As <sub>2</sub> CaGa <sub>2</sub> , Bi <sub>2</sub> PbTe <sub>4</sub> , AgGeLi <sub>2</sub> , PtTe, Bi <sub>2</sub> Se <sub>3</sub> , Bi <sub>2</sub> SeTe <sub>2</sub> , SbTe <sub>2</sub> Tl, Bi <sub>2</sub> Te <sub>3</sub> , CaGe <sub>2</sub> , Sb <sub>2</sub> SeTe <sub>2</sub> , Sb <sub>2</sub> Te <sub>3</sub> , Li <sub>8</sub> Pb <sub>3</sub> , Sb <sub>2</sub> SnTe <sub>4</sub> , C <sub>3</sub> Al <sub>6</sub> N <sub>2</sub> , Ba <sub>2</sub> Mg <sub>17</sub> , Nb <sub>6</sub> Zn <sub>7</sub> , C <sub>5</sub> Ti <sub>8</sub> , As <sub>2</sub> Ge <sub>4</sub> Te <sub>7</sub> , Pt <sub>2</sub> Te <sub>3</sub> , Cl <sub>8</sub> Na <sub>2</sub> Ti <sub>3</sub> , Sb <sub>8</sub> Te <sub>3</sub> , Al <sub>10</sub> Ba <sub>7</sub> , Bi <sub>6</sub> PbTe <sub>10</sub> , Bi <sub>8</sub> Te <sub>9</sub> , Sb <sub>48</sub> Te <sub>9</sub> , ClLa,
<b>167</b>	Pd <sub>8</sub> Sb <sub>3</sub> , Mo <sub>15</sub> Se <sub>19</sub> , Mo <sub>15</sub> Se <sub>19</sub> Tl <sub>2</sub> , Cd <sub>2</sub> Mo <sub>15</sub> Se <sub>19</sub> ,
<b>176</b>	Ba <sub>4</sub> Nb <sub>2</sub> O <sub>9</sub> ,
<b>191</b>	B <sub>2</sub> Sr, BaSi <sub>2</sub> , CaSi <sub>2</sub> , Li <sub>2</sub> Pd, CaZn <sub>5</sub> , Li <sub>2</sub> Pt, CaPd <sub>5</sub> , BaSn <sub>5</sub> , Ti, FN <sub>3</sub> Ta <sub>2</sub> , Ti <sub>2</sub> Zr,
<b>193</b>	Ca <sub>10</sub> Ge <sub>3</sub> Pt <sub>7</sub> , Ca <sub>10</sub> Pt <sub>7</sub> Si <sub>3</sub> , Pb <sub>3</sub> TeZr <sub>5</sub> ,
<b>194</b>	Zn, SnTi <sub>3</sub> , ScZn <sub>2</sub> , TaZn <sub>2</sub> , AgSbSr, AlN <sub>3</sub> Nb <sub>4</sub> , AuBaBi, CNb <sub>2</sub> Sn, CNb <sub>2</sub> S, Cd, BaSe <sub>3</sub> Ti, Ca <sub>2</sub> IN, InPt <sub>2</sub> Y, CaGaSn, Mg <sub>17</sub> Sr <sub>2</sub> , Ca <sub>4</sub> Mg <sub>13</sub> Zn <sub>29</sub> , Pt <sub>2</sub> SnU, LuMg <sub>2</sub> , Re <sub>2</sub> Y, AlN <sub>3</sub> Ti <sub>4</sub> , Al <sub>2</sub> Hf, C <sub>2</sub> AlTa <sub>3</sub> , MgPo, SiSr <sub>2</sub> ,
<b>200</b>	Cl <sub>7</sub> Na, Mg <sub>2</sub> Zn <sub>11</sub> , Cd <sub>11</sub> Na <sub>2</sub> ,
<b>204</b>	BaGe <sub>12</sub> Pt <sub>4</sub> ,
<b>205</b>	AgPd <sub>3</sub> Se, N <sub>2</sub> W, PdSb <sub>2</sub> , S <sub>2</sub> Ti,
<b>206</b>	Cd <sub>3</sub> N <sub>2</sub> , N <sub>2</sub> Zn <sub>3</sub> ,
<b>215</b>	Au <sub>9</sub> In <sub>4</sub> ,
<b>216</b>	AgKO, AgN, AgNaO, AgORb, AuGaLi <sub>2</sub> , HgS, InN, NTL, Pd <sub>17</sub> Te <sub>4</sub> , Au <sub>10</sub> Mo <sub>4</sub> Zn <sub>89</sub> , PtSnU, Pt <sub>5</sub> U, InLaPt <sub>4</sub> , NRe,
<b>221</b>	MgPd, PbSe, SnTe, AlSc, AlY, B <sub>6</sub> Ba, B <sub>6</sub> Ca, B <sub>6</sub> Sr, BeTi, Br <sub>3</sub> CsGe, Br <sub>3</sub> CsPb, CsI <sub>3</sub> Sn, Sn <sub>3</sub> U, HgTi <sub>3</sub> ,
<b>223</b>	BiNb <sub>3</sub> , HgTi <sub>3</sub> , HgZr <sub>3</sub> , Nb <sub>3</sub> Sb, SbTa <sub>3</sub> , SbTa <sub>3</sub> ,
<b>225</b>	HgP <sub>2</sub> Si, W, N <sub>2</sub> Pd, Li <sub>2</sub> MgSi, Y <sub>6</sub> Zn <sub>23</sub> , In <sub>7</sub> Sr <sub>11</sub> , BiY, CPd, CZr, Ca <sub>7</sub> Ge, Ca <sub>3</sub> Cd <sub>8</sub> Pt <sub>4</sub> , BiLu, BiLa, SeU, NPa, LaP, GeTh, LaSb, TeU, Ga <sub>4</sub> In <sub>3</sub> Sr <sub>11</sub> , AsLa,
<b>227</b>	CTi <sub>2</sub> , CTi, In <sub>2</sub> Mg, Se, Hf <sub>2</sub> Pd, Hf <sub>3</sub> NZn <sub>3</sub> , Al <sub>18</sub> Mg <sub>3</sub> W <sub>2</sub> , Al <sub>18</sub> Mg <sub>3</sub> Mo <sub>2</sub> , C <sub>3</sub> Nb <sub>8</sub> Zn <sub>4</sub> , Al <sub>2</sub> Th, CNb <sub>4</sub> Zn <sub>2</sub> ,

Part 5 of all the predicted TIs:

**229** | Be,

Part 1 of all the predicted TCIs:

TABLE VI. All the topological crystalline insulators: Note that, due to band dispersions these materials might not be insulating in reality.

SG	Topological crystalline insulators
<b>2</b>	AsF <sub>6</sub> N <sub>2</sub> S <sub>3</sub> , Br <sub>3</sub> Ti, Cl <sub>18</sub> Mo <sub>2</sub> P <sub>2</sub> , Cl <sub>5</sub> Mo, CsHg, Cl <sub>9</sub> TeW, HgK, K <sub>3</sub> Nb <sub>7</sub> O <sub>19</sub> , Mo <sub>6</sub> Se <sub>8</sub> Ti, O <sub>4</sub> PbPt <sub>2</sub> , STa <sub>6</sub> , O <sub>20</sub> SrTi <sub>11</sub> ,
<b>11</b>	Sb <sub>2</sub> Sr, Se <sub>3</sub> Ta, BaBi <sub>2</sub> Pd <sub>2</sub> , BaSb <sub>2</sub> , Bi <sub>2</sub> Pd <sub>2</sub> Sr, Li <sub>4</sub> S <sub>4</sub> Si, MoTe <sub>2</sub> , Pt <sub>6</sub> Si <sub>5</sub> , Pt <sub>3</sub> Ta, Ba <sub>3</sub> Ge <sub>2</sub> N <sub>2</sub> ,
<b>12</b>	As <sub>2</sub> Nb, As <sub>2</sub> Ta, Al <sub>14</sub> Ca <sub>13</sub> , As <sub>3</sub> Mo <sub>2</sub> , As <sub>3</sub> W <sub>2</sub> , As <sub>4</sub> Ba <sub>3</sub> Zn <sub>2</sub> , As <sub>4</sub> Zr <sub>7</sub> , Al <sub>4</sub> Na <sub>4</sub> P <sub>12</sub> Sr <sub>8</sub> , As <sub>4</sub> Hf <sub>7</sub> , AsF <sub>6</sub> NO <sub>2</sub> , Al <sub>4</sub> Cl <sub>51</sub> Zr <sub>12</sub> , BaPt <sub>2</sub> Sb <sub>2</sub> , Ba <sub>3</sub> Cd <sub>2</sub> Sb <sub>4</sub> , BiHf <sub>2</sub> , BiSe, BiBr, Bi <sub>2</sub> ITe, C <sub>5</sub> Nb <sub>6</sub> , ClZr, Br <sub>5</sub> W, Cl <sub>8</sub> NSc <sub>5</sub> , CdK <sub>6</sub> Pb <sub>8</sub> , Hf <sub>2</sub> Te, Hf <sub>7</sub> P <sub>4</sub> , In <sub>4</sub> Sr, LiMoO <sub>2</sub> , NbP <sub>2</sub> , NbSb <sub>2</sub> , Nb <sub>2</sub> Se, Nb <sub>7</sub> P <sub>4</sub> , O <sub>5</sub> Ti <sub>5</sub> , P <sub>4</sub> Zr <sub>7</sub> , Pt <sub>2</sub> Te <sub>3</sub> , Sb <sub>2</sub> Ta, Se <sub>4</sub> Ti <sub>3</sub> , Ta <sub>2</sub> Te <sub>3</sub> , Te <sub>4</sub> Ti <sub>3</sub> , Se <sub>3</sub> Ti <sub>8</sub> , LaSi <sub>5</sub> , Ge <sub>2</sub> Re, I <sub>3</sub> La <sub>5</sub> Si <sub>5</sub> ,
<b>13</b>	FMo <sub>2</sub> O <sub>7</sub> Y,
<b>14</b>	AsSeY, AsSY, LaSbSe, AsLuSe, K <sub>2</sub> O <sub>7</sub> W <sub>2</sub> , O <sub>7</sub> Si <sub>2</sub> Y <sub>2</sub> , O <sub>7</sub> Rb <sub>2</sub> W <sub>2</sub> , O <sub>7</sub> P <sub>2</sub> Sn <sub>2</sub> ,
<b>15</b>	P <sub>2</sub> Pt <sub>5</sub> , Sb <sub>2</sub> Te <sub>3</sub> , Na <sub>6</sub> Sb <sub>4</sub> Tl, Pb <sub>9</sub> Pd <sub>13</sub> ,
<b>47</b>	OTa <sub>4</sub> , MoO <sub>36</sub> W <sub>11</sub> ,
<b>51</b>	CdMg, BiPd <sub>3</sub> , MoPt, PdT <sub>i</sub> , GaPt <sub>2</sub> , BLi, C <sub>3</sub> AlY <sub>3</sub> , O <sub>5</sub> U <sub>2</sub> , Ca <sub>5</sub> P <sub>6</sub> Pd <sub>6</sub> ,
<b>55</b>	Ca <sub>5</sub> Ga <sub>2</sub> Sb <sub>6</sub> , Cd <sub>7</sub> Th <sub>6</sub> , B <sub>6</sub> ReY <sub>2</sub> , B <sub>6</sub> ReSc <sub>2</sub> , Ga <sub>2</sub> Mg, Bi <sub>8</sub> Ca <sub>3</sub> Pd <sub>4</sub> , C <sub>5</sub> Y <sub>4</sub> ,
<b>57</b>	Ca <sub>3</sub> Ga <sub>2</sub> Pd <sub>2</sub> , AlLu, Ca <sub>3</sub> Ga <sub>2</sub> Pt <sub>2</sub> ,
<b>58</b>	Bi <sub>3</sub> RbS <sub>5</sub> , STi <sub>2</sub> , P <sub>9</sub> Zr <sub>14</sub> , AsTa <sub>2</sub> ,
<b>59</b>	BrNTi, Ba <sub>6</sub> Ge <sub>5</sub> N <sub>2</sub> , INTi, PdSiY,
<b>61</b>	O <sub>2</sub> U,
<b>62</b>	BiI <sub>3</sub> , Ga <sub>5</sub> Y <sub>3</sub> , PSc <sub>3</sub> , PdSn, PdSi, Pd <sub>2</sub> Sn, PtSc <sub>2</sub> , GePd, GePt, Sb <sub>3</sub> Sc <sub>5</sub> , CaTe, Ge <sub>2</sub> Pt <sub>3</sub> , Ca <sub>3</sub> Hg, HgSr <sub>3</sub> , In <sub>5</sub> Y <sub>3</sub> , Ca <sub>7</sub> Ge <sub>6</sub> , MgSi <sub>2</sub> Sr, MoPt <sub>3</sub> Si <sub>4</sub> , SiU, LaSbTe, Te <sub>5</sub> U, Ga <sub>5</sub> Lu <sub>3</sub> , In <sub>4</sub> La <sub>2</sub> Pd <sub>3</sub> , Lu <sub>5</sub> Sb <sub>3</sub> , PtY <sub>2</sub> ,
<b>63</b>	AlGeSc, AlSiY, AsIn, AuY, BaGe, BaSi, BaSn, BaSi <sub>6</sub> , Bi <sub>2</sub> Ca, Au <sub>3</sub> Mg, CaGe, CaIn <sub>2</sub> Pd, CaIn <sub>2</sub> Pt, Ba <sub>3</sub> Pb <sub>5</sub> , CaSn, CaPdSn <sub>2</sub> , Ca <sub>3</sub> Zn, Ge <sub>2</sub> Pt <sub>3</sub> , HgTe, In <sub>2</sub> PdSr, Cd <sub>2</sub> FSb <sub>5</sub> Sr <sub>5</sub> , PdSrTl <sub>2</sub> , PbSr, SnSr, Pd <sub>3</sub> Te <sub>2</sub> , Si <sub>2</sub> Ti, Si <sub>6</sub> Sr, Ba <sub>5</sub> Cd <sub>2</sub> FSb <sub>5</sub> , AlGeLu, AlLuSi, N <sub>3</sub> TaTh, La <sub>2</sub> Li <sub>2</sub> Si <sub>3</sub> , La <sub>2</sub> PbZn <sub>5</sub> , Ge <sub>3</sub> La <sub>2</sub> Li <sub>2</sub> , La <sub>3</sub> Tl <sub>5</sub> , Al <sub>2</sub> GeLa <sub>2</sub> , CsScSe <sub>5</sub> U, Al <sub>4</sub> Mg <sub>19</sub> Zn <sub>15</sub> , BaPb, Ca <sub>2</sub> InN, In <sub>5</sub> Y <sub>3</sub> ,
<b>64</b>	BiSn, Ba <sub>2</sub> Ge <sub>4</sub> Pd <sub>5</sub> , Li, Ca <sub>5</sub> Ga <sub>2</sub> N <sub>4</sub> , LaS,
<b>65</b>	INaO <sub>3</sub> , Au <sub>7</sub> Rb <sub>3</sub> , Ba <sub>3</sub> Nb <sub>16</sub> O <sub>23</sub> , Ba <sub>4</sub> Nb <sub>14</sub> O <sub>23</sub> , La <sub>2</sub> Sn <sub>5</sub> , In <sub>9</sub> La <sub>11</sub> Pd <sub>4</sub> , OTi <sub>2</sub> Zr, Ga <sub>13</sub> Nb <sub>5</sub> ,
<b>69</b>	Ag <sub>2</sub> Ca <sub>4</sub> Si <sub>6</sub> , Bi <sub>2</sub> CaNb <sub>2</sub> O <sub>9</sub> , Ge <sub>6</sub> Li <sub>2</sub> Sr <sub>4</sub> , K <sub>2</sub> Pd <sub>3</sub> S <sub>6</sub> U, Pd <sub>3</sub> Rb <sub>2</sub> Se <sub>6</sub> U, Cs <sub>2</sub> Pd <sub>3</sub> Se <sub>6</sub> U,
<b>71</b>	Al <sub>2</sub> Ca <sub>3</sub> Ge <sub>2</sub> , Ca <sub>2</sub> CdPd <sub>2</sub> , Ca <sub>2</sub> MgPd <sub>2</sub> , Ca <sub>2</sub> MgPt <sub>2</sub> , HgO <sub>6</sub> Pt <sub>3</sub> , Ge <sub>2</sub> PtY, Li <sub>4</sub> Sb <sub>4</sub> Sr <sub>3</sub> , Al <sub>4</sub> OSi <sub>6</sub> Sr <sub>10</sub> , B <sub>4</sub> Ti <sub>3</sub> , Ba <sub>3</sub> Bi <sub>4</sub> Li <sub>4</sub> , Ba <sub>3</sub> Li <sub>4</sub> Sb <sub>4</sub> , Ba <sub>3</sub> CdHg <sub>10</sub> , Sn <sub>5</sub> Ti <sub>6</sub> ,
<b>72</b>	Pt <sub>3</sub> Sb <sub>2</sub> , Mg <sub>5</sub> Tl <sub>2</sub> , Pt <sub>5</sub> Ti <sub>3</sub> , Ge <sub>5</sub> Ti <sub>6</sub> ,

Part 2 of all the predicted TCIs:

<b>73</b>	AlLi <sub>3</sub> P <sub>2</sub> ,
<b>74</b>	BaCd <sub>2</sub> , CaCd <sub>2</sub> , Hg <sub>2</sub> Sr, BaZn <sub>2</sub> , CaZn <sub>2</sub> , BaHg <sub>2</sub> , SrZn <sub>2</sub> , Cd <sub>2</sub> Sr, BaGe <sub>5</sub> ,
<b>84</b>	P <sub>2</sub> S <sub>6</sub> U,
<b>85</b>	P <sub>2</sub> U,
<b>86</b>	SiTa <sub>3</sub> ,
<b>87</b>	Au <sub>4</sub> Ti,
<b>88</b>	O <sub>4</sub> PbPd <sub>2</sub> , P <sub>4</sub> S <sub>12</sub> U,
<b>123</b>	AsNa, CdHg <sub>2</sub> Ti, Pd <sub>3</sub> Sn, Pb <sub>3</sub> Sr, CPd <sub>3</sub> Sn, As <sub>3</sub> RbZn <sub>4</sub> , Pt <sub>5</sub> SiSn, As <sub>3</sub> CsZn <sub>4</sub> , BaOSb <sub>2</sub> Ti <sub>2</sub> , AgSbTe <sub>2</sub> ,
<b>127</b>	Pb <sub>3</sub> Sr <sub>2</sub> , Li <sub>2</sub> Sn <sub>5</sub> , B <sub>4</sub> Ca, Si <sub>2</sub> U <sub>3</sub> ,
<b>129</b>	GeSzr, GeNbSb, SnTeZr, OSiZr, SeSiZr, SSiZr, SiTeZr, HfSSI, GeSeZr, HfSeSi, GeHfSe, GeHfS, GeHfTe, AsGeNb, BaPd <sub>2</sub> Sb <sub>2</sub> , Pd <sub>2</sub> Sb <sub>2</sub> Sr, Bi <sub>2</sub> Pd <sub>2</sub> Sr, Au <sub>2</sub> Ga <sub>2</sub> Sr, BaMg <sub>2</sub> Pb <sub>2</sub> , BaMg <sub>2</sub> Sn <sub>2</sub> , CsF <sub>4</sub> Ti, BiO <sub>3</sub> Te, In <sub>9</sub> Li <sub>2</sub> Y <sub>5</sub> , Al <sub>2</sub> Au <sub>2</sub> Th, As <sub>2</sub> U, As <sub>2</sub> PdU, GeSU, P <sub>2</sub> U, SSiU, SnTeU, Sb <sub>2</sub> U, Pt <sub>2</sub> Si <sub>2</sub> Th, LaSbTe, PdSb <sub>2</sub> U, HfSiTe,
<b>136</b>	Al <sub>2</sub> Hf <sub>3</sub> , Al <sub>2</sub> Lu <sub>3</sub> ,
<b>137</b>	Ba <sub>2</sub> LiN,
<b>139</b>	As <sub>2</sub> Pd <sub>2</sub> Sr, As <sub>2</sub> CaPd <sub>2</sub> , BePd <sub>2</sub> , Ba <sub>2</sub> Zn, CaGe <sub>2</sub> Pd <sub>2</sub> , Au <sub>2</sub> CaGe <sub>2</sub> , AsTiZr, Ba <sub>2</sub> Cd, BaPd <sub>2</sub> Sb <sub>2</sub> , Ba <sub>2</sub> Hg, AsCa <sub>2</sub> , CaPd <sub>2</sub> Si <sub>2</sub> , Al <sub>3</sub> Hf, Pd <sub>2</sub> Sb <sub>2</sub> Sr, ZnZr <sub>2</sub> , Ag <sub>2</sub> BaSn <sub>2</sub> , Hf <sub>2</sub> Hg, Br <sub>2</sub> Ca <sub>3</sub> Si, BiSr <sub>2</sub> , AsBa <sub>2</sub> , SbZr <sub>2</sub> , Pd <sub>2</sub> Si <sub>2</sub> Sr, Ga <sub>4</sub> Ti <sub>2</sub> Zr, SbYZr, CaIn, MoO <sub>4</sub> Sr <sub>2</sub> , Ba <sub>2</sub> Bi, SbSr <sub>2</sub> , Bi <sub>2</sub> F <sub>2</sub> OSr <sub>2</sub> Ti <sub>2</sub> , As <sub>2</sub> F <sub>2</sub> OSr <sub>2</sub> Ti <sub>2</sub> , CaSi <sub>3</sub> , Si <sub>3</sub> Y, Ba <sub>2</sub> Sb, F <sub>2</sub> OSb <sub>2</sub> Sr <sub>2</sub> Ti <sub>2</sub> , Ca <sub>2</sub> Pd <sub>3</sub> Sb <sub>4</sub> , Al <sub>2</sub> Ge <sub>8</sub> Sc <sub>11</sub> , Ga <sub>10</sub> Hf <sub>11</sub> , Au <sub>2</sub> Si <sub>2</sub> U, Ge <sub>2</sub> Pd <sub>2</sub> Th, Ge <sub>2</sub> Pt <sub>2</sub> Th, Ge <sub>2</sub> Pt <sub>2</sub> U, ThZn <sub>4</sub> , GeLaSc, Pd <sub>2</sub> Si <sub>2</sub> Th, LaScSi, Pt <sub>2</sub> Th, PTeU, Pt <sub>2</sub> Si <sub>2</sub> Th, O <sub>4</sub> Te <sub>3</sub> U <sub>4</sub> , Ge <sub>4</sub> In <sub>6</sub> La <sub>11</sub> , Ti <sub>2</sub> Zn, Hf <sub>2</sub> Zn, CdHf <sub>2</sub> , Ag <sub>2</sub> BaGe <sub>2</sub> , BaSi <sub>2</sub> , Ca <sub>2</sub> Sb, K <sub>2</sub> Mg <sub>5</sub> Sn <sub>3</sub> , Mo <sub>3</sub> Sb <sub>7</sub> ,
<b>140</b>	Bi, Mg <sub>2</sub> Pt, MoO <sub>3</sub> Sr, GePt <sub>3</sub> , GeNb <sub>3</sub> , Ca <sub>5</sub> Hg <sub>3</sub> , Cd <sub>3</sub> Sr <sub>5</sub> , Ga <sub>2</sub> Sc <sub>3</sub> , Ga <sub>2</sub> Y <sub>3</sub> , Ga <sub>2</sub> Lu <sub>3</sub> , Lu <sub>7</sub> Sb <sub>3</sub> ,
<b>141</b>	Al <sub>2</sub> Mg,
<b>147</b>	Bi <sub>2</sub> Pt,
<b>148</b>	Mo <sub>6</sub> S <sub>8</sub> , Mo <sub>18</sub> S <sub>22</sub> Tl <sub>4</sub> , Mo <sub>3</sub> S <sub>4</sub> ,
<b>164</b>	BaSi <sub>2</sub> , CW <sub>2</sub> , B <sub>2</sub> O, Bi <sub>2</sub> Pb <sub>2</sub> Te <sub>5</sub> , Bi <sub>2</sub> Se <sub>2</sub> , BiTe, Bi <sub>3</sub> STe <sub>2</sub> , CdO <sub>4</sub> S, Te <sub>2</sub> Zr, HgPt <sub>2</sub> Se <sub>3</sub> , AlLaSi <sub>2</sub> ,
<b>166</b>	Bi, B <sub>2</sub> Mo, ClZr, Hg, CNb <sub>2</sub> S <sub>2</sub> , BrZr, P, Ba <sub>3</sub> O <sub>9</sub> Sc <sub>4</sub> , B <sub>4</sub> Mo <sub>2</sub> , AsNaTe <sub>2</sub> Zr <sub>2</sub> , Ag <sub>4</sub> Sb <sub>2</sub> Sr, TeZr <sub>3</sub> , Ga, As <sub>3</sub> Cd <sub>4</sub> Na, As <sub>3</sub> Cd <sub>4</sub> K, Pd <sub>3</sub> S <sub>2</sub> Tl <sub>2</sub> , Bi <sub>4</sub> Se <sub>3</sub> , As <sub>3</sub> Cd <sub>4</sub> Rb, Pt <sub>3</sub> Te <sub>4</sub> , Bi <sub>8</sub> Se <sub>9</sub> , BrLa, C <sub>6</sub> Al <sub>4</sub> Hf <sub>3</sub> ,

Part 3 of all the predicted TCIs:

<b>176</b>	Mo <sub>9</sub> Se <sub>11</sub> , Mo <sub>15</sub> S <sub>19</sub> ,
<b>187</b>	CHf, NbSe <sub>2</sub> , NY, InNbS <sub>2</sub> , PPtY, InNbSe <sub>2</sub> , Br <sub>2</sub> Ca <sub>3</sub> Si, LuPPt,
<b>189</b>	AgGeSc, CaPbPd, CaCdPb, AgPbY, AgAsCa, GaMgY, MgTiY, AlMgY, GePdTi, CaCdGe, CaCdSn, GeLiY, InMgY, BLiPt <sub>3</sub> , Rb <sub>15</sub> Tl <sub>27</sub> , CsRb <sub>14</sub> Tl <sub>27</sub> , InLaPt, AsLuPd, AuCdLa, Ge <sub>3</sub> La <sub>2</sub> Zn <sub>6</sub> , LaMgTl, AgCaP, AgMgY, AuGaMg, AgSiY, LiSiY, OTi, Pt <sub>5</sub> Th <sub>3</sub> , PtSnU, Pd <sub>5</sub> Th <sub>3</sub> , Se <sub>2</sub> U, GaLaMg, AgLuSi, AgLaMg, Os <sub>8</sub> U <sub>3</sub> ,
<b>191</b>	B <sub>2</sub> Mg, B <sub>2</sub> Ti, B <sub>2</sub> Ca, B <sub>2</sub> Zr, C <sub>2</sub> Ca, Ga <sub>2</sub> Sr, Si, Pd <sub>5</sub> Sr, Be <sub>12</sub> Ti,
<b>193</b>	Pb <sub>3</sub> SZr <sub>5</sub> , NbSb <sub>5</sub> U <sub>3</sub> ,
<b>194</b>	SnTi <sub>2</sub> , AlLi, AsHgK, B <sub>2</sub> W, C, CGeNb <sub>2</sub> , CCdTi <sub>2</sub> , CdNa <sub>2</sub> Sn, HgKSb, BaGaGe, Cs <sub>3</sub> I <sub>9</sub> Mo <sub>2</sub> , Mg <sub>4</sub> Sr, ILa, I <sub>2</sub> Th, Hf <sub>9</sub> Re <sub>4</sub> Se, Hf <sub>9</sub> Re <sub>4</sub> S, AsPtY,
<b>204</b>	Al <sub>12</sub> Mo, Al <sub>12</sub> W, NPd <sub>3</sub> ,
<b>221</b>	NY, NTi <sub>3</sub> Tl, PbPt <sub>3</sub> , Pt <sub>3</sub> Sn, Pt <sub>3</sub> Zn, AgGa, AgIn, AgLi, AlAu, CPbPd <sub>3</sub> , CPt <sub>3</sub> Sn, C <sub>3</sub> Nb <sub>4</sub> , CaPd, Ca <sub>3</sub> GeO, Ca <sub>3</sub> OPb, HfPd <sub>3</sub> , HgPt <sub>3</sub> , CTh, LaN, N <sub>3</sub> TaTh, SiU <sub>3</sub> , Ca <sub>3</sub> OSn, OSnSr <sub>3</sub> , OPbSr <sub>3</sub> , Ba <sub>3</sub> OPb,
<b>225</b>	PbPo, SSn, SbSc, SeSn, SnTe, Ag <sub>2</sub> MgZn, AlAu <sub>2</sub> Sc, Al <sub>2</sub> O, AsSc, Au <sub>2</sub> InSc, Au <sub>2</sub> InY, B <sub>12</sub> Hf, Au <sub>2</sub> Cl <sub>6</sub> Cs <sub>2</sub> , Ba, BiI <sub>3</sub> , BiSc, CPt, Ca, Au <sub>2</sub> InLu, B <sub>12</sub> Th, O <sub>2</sub> U, LuSb, CW, Al <sub>16</sub> Pt <sub>7</sub> Zr <sub>6</sub> ,
<b>227</b>	Al <sub>2</sub> Sr, Al <sub>2</sub> Ba, S <sub>2</sub> Ti, Pd <sub>13</sub> Te <sub>3</sub> , Mo <sub>2</sub> O <sub>7</sub> Y <sub>2</sub> , Ba <sub>21</sub> O <sub>5</sub> Si <sub>2</sub> , La <sub>2</sub> O <sub>7</sub> Zr <sub>2</sub> , Cd <sub>2</sub> O <sub>7</sub> Re <sub>2</sub> , HfZn <sub>2</sub> , NPd <sub>2</sub> Zr <sub>4</sub> ,

Part 1 of all the predicted **Case 3**-TSMs:

TABLE VII. All the topological (semi-)metals from **Case 3**.

<i>SG</i>	Topological (semi-)metals
<b>2</b>	AgF <sub>11</sub> NaZr <sub>2</sub> , AgBi <sub>2</sub> F <sub>12</sub> , AgF <sub>6</sub> Sn, AgF <sub>12</sub> Sb <sub>2</sub> , AgF <sub>6</sub> Ti, AgF <sub>12</sub> Ta <sub>2</sub> , As <sub>10</sub> Cs <sub>13</sub> In <sub>6</sub> Nb <sub>2</sub> , Ba <sub>14</sub> CaN <sub>6</sub> Na <sub>17</sub> , Cl <sub>6</sub> ISe <sub>6</sub> W, Cl <sub>8</sub> NW <sub>2</sub> , InMo <sub>6</sub> S <sub>8</sub> , I <sub>10</sub> Ta <sub>7</sub> Te <sub>24</sub> , Cl <sub>12</sub> ReTe <sub>2</sub> , Se <sub>2</sub> Ta,
<b>4</b>	Ge <sub>2</sub> Pt <sub>2</sub> Y,
<b>5</b>	F <sub>11</sub> I <sub>2</sub> Sb <sub>2</sub> , NbS <sub>2</sub> , I <sub>47</sub> W <sub>15</sub> ,
<b>6</b>	Mo <sub>8</sub> P <sub>5</sub> ,
<b>10</b>	AuCd,
<b>11</b>	S <sub>3</sub> Ta, BeLi, CBrHgNS, Bi <sub>9</sub> I <sub>2</sub> , Br <sub>9</sub> TeW, Li <sub>7</sub> Sn <sub>3</sub> , Ge <sub>6</sub> Pt <sub>4</sub> Y <sub>3</sub> , Mo <sub>2</sub> S <sub>2</sub> Sb, NbS <sub>3</sub> , Pd <sub>3</sub> Ta <sub>3</sub> Te <sub>14</sub> , N <sub>2</sub> Re, CBCl <sub>3</sub> La <sub>3</sub> ,
<b>12</b>	AlMg <sub>4</sub> Si <sub>6</sub> , AgMo <sub>6</sub> Te <sub>6</sub> , Al <sub>3</sub> Si <sub>2</sub> Y <sub>2</sub> , AgBi <sub>6</sub> S <sub>9</sub> , Al <sub>4</sub> Li <sub>9</sub> , Ag <sub>3</sub> F <sub>14</sub> Hf <sub>2</sub> , As <sub>4</sub> Na <sub>5</sub> , Bi <sub>8</sub> I <sub>3</sub> Pt <sub>5</sub> , Cl <sub>5</sub> Y <sub>4</sub> , CCl <sub>8</sub> Sc <sub>5</sub> , C <sub>2</sub> Cl <sub>10</sub> Sc <sub>7</sub> , C <sub>2</sub> I <sub>7</sub> Y <sub>6</sub> , Cl <sub>10</sub> Sc <sub>7</sub> , Ba <sub>14</sub> CaN <sub>6</sub> Na <sub>21</sub> , Cl <sub>8</sub> Sc <sub>5</sub> , Cl <sub>6</sub> O <sub>2</sub> TlW <sub>2</sub> , CsSe <sub>8</sub> Ti <sub>5</sub> , CsTe <sub>8</sub> Ti <sub>5</sub> , Ga <sub>3</sub> Pd <sub>7</sub> , Ga <sub>5</sub> Pd <sub>13</sub> , InPt, KSe <sub>8</sub> Ti <sub>5</sub> , K <sub>5</sub> Sb <sub>4</sub> , In <sub>9</sub> Pt <sub>13</sub> , Mo <sub>2</sub> O <sub>12</sub> Y <sub>5</sub> , NaSe <sub>8</sub> Ti <sub>5</sub> , NbTe <sub>2</sub> , Nb <sub>5</sub> PbSe <sub>8</sub> , Nb <sub>5</sub> Se <sub>8</sub> Sr, Nb <sub>5</sub> Se <sub>8</sub> Sn, Na <sub>3</sub> O <sub>13</sub> Ti <sub>6</sub> , O <sub>3</sub> Sr <sub>2</sub> Tl, RbSe <sub>8</sub> Ti <sub>5</sub> , S <sub>7</sub> Y <sub>5</sub> , TaTe <sub>2</sub> , Se <sub>8</sub> Ti <sub>5</sub> Tl, P <sub>4</sub> Re <sub>3</sub> , In <sub>21</sub> Pd <sub>10</sub> Th <sub>4</sub> , O <sub>64</sub> P <sub>8</sub> Rb <sub>2</sub> W <sub>16</sub> , N <sub>2</sub> Re,
<b>13</b>	F <sub>6</sub> ISbSe <sub>6</sub> ,
<b>14</b>	MgP <sub>4</sub> , F <sub>4</sub> Xe, CdP <sub>4</sub> , InS, NS, F <sub>4</sub> Na <sub>2</sub> Pd, Cl <sub>2</sub> PdSe <sub>6</sub> , F <sub>6</sub> Li <sub>2</sub> Pt, ClII, Br <sub>6</sub> Pb <sub>2</sub> Pd, O <sub>6</sub> Se <sub>2</sub> Sn, Cl <sub>6</sub> Pb <sub>2</sub> Pd, F <sub>6</sub> Na <sub>2</sub> Sn, C <sub>2</sub> Li <sub>2</sub> O <sub>4</sub> , C <sub>2</sub> CdO <sub>4</sub> , C <sub>60</sub> Na <sub>2</sub> Rb, N <sub>2</sub> O <sub>4</sub> , F <sub>8</sub> Sn <sub>3</sub> , C <sub>2</sub> Na <sub>2</sub> O <sub>4</sub> , O <sub>3</sub> Rb, F <sub>8</sub> Ge <sub>3</sub> , C <sub>2</sub> Ag <sub>2</sub> O <sub>4</sub> , K <sub>2</sub> MgP <sub>2</sub> Se <sub>6</sub> , CdP <sub>2</sub> Rb <sub>2</sub> Se <sub>6</sub> , C <sub>2</sub> O <sub>4</sub> Tl <sub>2</sub> , Cl <sub>8</sub> PtS <sub>2</sub> , Cl <sub>3</sub> MoO, Cs <sub>2</sub> I <sub>8</sub> , C <sub>4</sub> Na <sub>2</sub> O <sub>4</sub> , Cl <sub>6</sub> HfHg <sub>3</sub> Se <sub>2</sub> , Al <sub>2</sub> Cl <sub>8</sub> Ti, AuBr <sub>4</sub> Rb, AuGa <sub>2</sub> , Al <sub>2</sub> Cl <sub>8</sub> Pd, Au <sub>3</sub> F <sub>8</sub> , Au <sub>4</sub> Ca <sub>5</sub> , AgP <sub>2</sub> , Ag <sub>3</sub> O <sub>4</sub> , B <sub>2</sub> F <sub>4</sub> , BBiO <sub>3</sub> , AsF <sub>6</sub> N <sub>2</sub> S <sub>3</sub> , As <sub>2</sub> La, Ge <sub>2</sub> LaPt <sub>2</sub> , O <sub>2</sub> Re,
<b>15</b>	LiO <sub>6</sub> Si <sub>2</sub> Ti, NaO <sub>6</sub> Si <sub>2</sub> Ti, RbTe <sub>6</sub> , BaI <sub>4</sub> La, I <sub>4</sub> LaSr, O <sub>6</sub> Re <sub>2</sub> Sb, BiO <sub>6</sub> Re <sub>2</sub> ,
<b>19</b>	P <sub>7</sub> Th,
<b>20</b>	Rb, Cs,
<b>25</b>	C <sub>7</sub> B,
<b>29</b>	N <sub>2</sub> Re,
<b>33</b>	I <sub>11</sub> Nb <sub>6</sub> ,
<b>36</b>	AsPb <sub>2</sub> Pd <sub>3</sub> , AsF <sub>9</sub> S, CAI <sub>4</sub> N <sub>3</sub> O,
<b>39</b>	LaS,
<b>43</b>	Al <sub>3</sub> Hf <sub>2</sub> , Al <sub>3</sub> Zr <sub>2</sub> , Ga <sub>3</sub> Zr <sub>2</sub> , Ga <sub>3</sub> Hf <sub>2</sub> , Ge <sub>5</sub> Y <sub>3</sub> , Cl <sub>12</sub> ReSe <sub>2</sub> , Ba <sub>5</sub> P <sub>9</sub> ,
<b>44</b>	C <sub>5</sub> B, LiO <sub>3</sub> , NaO <sub>3</sub> , Ca <sub>28</sub> Ga <sub>11</sub> , Al <sub>4</sub> La, Lu <sub>7</sub> Pd <sub>2</sub> Te <sub>2</sub> ,
<b>47</b>	NbO,
<b>51</b>	AuCd, AuTi, NbPt, AsNb <sub>2</sub> , CsTe <sub>5</sub> TiU, CsTe <sub>5</sub> UZr, CB <sub>2</sub> N, FLiNb <sub>6</sub> O <sub>15</sub> , Nb <sub>2</sub> P,

Part 2 of all the predicted **Case 3-TSMs**:

<b>52</b>	Ag <sub>2</sub> BiO <sub>3</sub> , Bi <sub>3</sub> Sr <sub>2</sub> ,
<b>55</b>	Al <sub>3</sub> Pd <sub>5</sub> , Al <sub>3</sub> Pt <sub>5</sub> , In <sub>3</sub> Pd <sub>5</sub> , In <sub>4</sub> Pd <sub>2</sub> Y <sub>5</sub> , Bi <sub>9</sub> Ca <sub>9</sub> Cd <sub>4</sub> , In <sub>9</sub> Pb <sub>4</sub> S <sub>17</sub> , Bi <sub>9</sub> Cd <sub>4</sub> Sr <sub>9</sub> , In <sub>5</sub> S <sub>13</sub> Y <sub>4</sub> , In <sub>4</sub> Lu <sub>5</sub> Pd <sub>2</sub> , In <sub>5</sub> La <sub>4</sub> S <sub>13</sub> , Ga <sub>3</sub> Pd <sub>5</sub> , Cl <sub>6</sub> NSc <sub>4</sub> , Bi <sub>9</sub> Ca <sub>9</sub> Zn <sub>4</sub> , BCl <sub>6</sub> Sc <sub>4</sub> , Ca <sub>9</sub> Sb <sub>9</sub> Zn <sub>4</sub> , KNb <sub>8</sub> O <sub>14</sub> ,
<b>56</b>	Cl <sub>6</sub> ReSe <sub>4</sub> ,
<b>57</b>	AlCaPd, Cs, BiK <sub>2</sub> Sn, Al <sub>3</sub> Ca <sub>4</sub> Mg, GaHf, Hg <sub>7</sub> K <sub>5</sub> , InTh, ThTl,
<b>58</b>	BPd <sub>2</sub> , AuN <sub>2</sub> , LiO <sub>2</sub> , AlAu <sub>2</sub> , NPd <sub>2</sub> , LiO <sub>2</sub> Tl, NaO <sub>2</sub> , Hf <sub>2</sub> P, Ba <sub>8</sub> PdSe <sub>16</sub> U <sub>2</sub> , Nb <sub>5</sub> O <sub>17</sub> Sr <sub>5</sub> , C <sub>60</sub> K,
<b>59</b>	NbPt <sub>3</sub> , Pt <sub>3</sub> Ta, ClLiNTi, BrOTi, NbPd <sub>3</sub> , C <sub>4</sub> I <sub>8</sub> OY <sub>9</sub> , Ag <sub>3</sub> Sn, Au <sub>3</sub> Hf, Au <sub>3</sub> Zr, Bi <sub>5</sub> K <sub>6</sub> Zn, AsPdZr, Ba <sub>7</sub> Ga <sub>4</sub> Sb <sub>9</sub> , Br <sub>3</sub> La <sub>6</sub> Si <sub>7</sub> ,
<b>60</b>	F <sub>4</sub> NaTi, S <sub>5</sub> U <sub>2</sub> , O <sub>2</sub> Re,
<b>61</b>	AgF <sub>2</sub> ,
<b>62</b>	InPdSr, AlCaPt, PtSnY, InPtSr, As <sub>2</sub> Sc <sub>3</sub> , AlGe <sub>3</sub> Y <sub>2</sub> , AgAlCsF <sub>6</sub> , AgAsF <sub>7</sub> , AlMgSi, AlPd <sub>2</sub> , AlAu <sub>2</sub> , Cs, AlAuY, AlY <sub>2</sub> , AlPt <sub>2</sub> , AsMo, AlPd <sub>5</sub> , AgSc <sub>6</sub> Te <sub>2</sub> , AgTe <sub>2</sub> Y <sub>6</sub> , AgSr, As <sub>3</sub> Ti <sub>5</sub> , FNanNbO <sub>2</sub> , Ba <sub>3</sub> I <sub>2</sub> P <sub>3</sub> , F <sub>5</sub> K <sub>2</sub> Ti, Bi <sub>3</sub> Ca <sub>5</sub> , Bi <sub>3</sub> Sr <sub>5</sub> , GaPd <sub>2</sub> , AgBa, C <sub>2</sub> MoY, PW, O <sub>3</sub> TiY, P <sub>2</sub> Sc <sub>3</sub> , AgF <sub>3</sub> K, C <sub>2</sub> WY, PPd <sub>3</sub> , PdSbZr, PdScSi, Pd <sub>2</sub> Tl, PdSnY, PdYZn, GeNbPt, PdY <sub>3</sub> , PtY, PtScSi, PtSiY, AgCaGe, Pd <sub>2</sub> SiY, GePd <sub>2</sub> Y, GePtSc, GePtY, Pt <sub>2</sub> SiY, Ge <sub>2</sub> LiSr, YZn <sub>3</sub> , PtSc <sub>3</sub> Si <sub>3</sub> , CaGaPt, P <sub>3</sub> Pd <sub>4</sub> Zr <sub>3</sub> , GeNb <sub>3</sub> Te <sub>6</sub> , CaInPd, CaInPt, CaGe <sub>2</sub> Li, Ge <sub>4</sub> Hf <sub>2</sub> Nb <sub>3</sub> , CaLiSi <sub>2</sub> , Si <sub>4</sub> Y <sub>5</sub> , Sb <sub>3</sub> Zr <sub>5</sub> , CaNbO <sub>3</sub> , Ge <sub>4</sub> Nb <sub>5</sub> , Ge <sub>4</sub> Nb <sub>3</sub> Zr <sub>2</sub> , Ge <sub>4</sub> Nb <sub>3</sub> Y <sub>2</sub> , Ge <sub>4</sub> Nb <sub>3</sub> Sc <sub>2</sub> , Ge <sub>4</sub> Hf <sub>4</sub> Nb, Ge <sub>4</sub> Sc <sub>5</sub> , CaPtSb, Ge <sub>4</sub> Y <sub>5</sub> , Ca <sub>2</sub> In, AgAuF <sub>7</sub> , Pt <sub>4</sub> Y <sub>5</sub> , Hg <sub>6</sub> K, Hf <sub>5</sub> Sb <sub>3</sub> , InPd <sub>2</sub> , Hf <sub>3</sub> P <sub>3</sub> Pd <sub>4</sub> , Hf <sub>3</sub> PdSb <sub>7</sub> , Ca <sub>5</sub> Sb <sub>3</sub> , SiTa <sub>3</sub> Te <sub>6</sub> , Sb <sub>3</sub> Sr <sub>5</sub> , PdSb <sub>7</sub> Zr <sub>3</sub> , N, N <sub>3</sub> Nb <sub>2</sub> , NaO <sub>4</sub> Ti <sub>2</sub> , NbO <sub>3</sub> Sr, NbPdSi, NbPtSi, NbPdTe <sub>5</sub> , Nb <sub>2</sub> P <sub>5</sub> , Nb <sub>3</sub> Sc <sub>2</sub> Si <sub>4</sub> , Nb <sub>3</sub> SiTe <sub>6</sub> , LaSi, LuPt, LaPdZn, GeLa, AuLu <sub>2</sub> , LaPtSn, LuPtSi, GeLuPt, LuPd <sub>2</sub> Si, LuZn <sub>3</sub> , GaPd <sub>2</sub> U, GeLaPd <sub>2</sub> , GeLuPd <sub>2</sub> , LaO <sub>3</sub> Ti, LaO <sub>3</sub> Pd, GeLa <sub>3</sub> , NaO <sub>3</sub> U, Lu <sub>3</sub> Pt, LuPt <sub>2</sub> Si, Au <sub>2</sub> In <sub>4</sub> La, Ge <sub>4</sub> Nb <sub>3</sub> U <sub>2</sub> , Ge <sub>4</sub> Lu <sub>2</sub> Nb <sub>3</sub> , Ge <sub>4</sub> Ta <sub>3</sub> U <sub>2</sub> , Ge <sub>4</sub> Lu <sub>5</sub> , Cl <sub>5</sub> K <sub>2</sub> U, Ge <sub>4</sub> La <sub>5</sub> , PRe <sub>2</sub> , Br <sub>5</sub> K <sub>2</sub> U, Cl <sub>5</sub> Rb <sub>2</sub> U, AuLu <sub>6</sub> Te <sub>2</sub> , AgLu <sub>6</sub> Te <sub>2</sub> , Lu <sub>5</sub> Pt <sub>4</sub> , La <sub>5</sub> Sn <sub>4</sub> , La <sub>5</sub> Pb <sub>4</sub> , Ba <sub>2</sub> O <sub>5</sub> Re, La <sub>3</sub> Pd <sub>4</sub> Sn <sub>6</sub> , La <sub>3</sub> MoO <sub>7</sub> , F <sub>8</sub> K <sub>2</sub> Re, P <sub>3</sub> Ti <sub>5</sub> , PtY <sub>3</sub> , Sb <sub>3</sub> Ti <sub>5</sub> , Pb <sub>4</sub> Y <sub>5</sub> , Sn <sub>4</sub> Y <sub>5</sub> , CsTe <sub>6</sub> U, Nb <sub>3</sub> Si,
<b>63</b>	AlHf, PdScZn, Ga <sub>2</sub> PdY, Ca <sub>3</sub> Tl <sub>5</sub> , In <sub>7</sub> K <sub>2</sub> Sr, AgCa, AlZr, AuCa, BMo, BW, Ag <sub>7</sub> Ca <sub>2</sub> , B <sub>3</sub> Nb <sub>2</sub> , BiZr, CBMo <sub>2</sub> , CaGa, C <sub>2</sub> B <sub>3</sub> Nb <sub>4</sub> , Cd <sub>3</sub> Y, Cd <sub>7</sub> Sc, GaLi <sub>2</sub> , GeSc, GeY, Ga <sub>3</sub> PdSr, Ge <sub>2</sub> Sc, Ca <sub>3</sub> Ga <sub>5</sub> , Ge <sub>3</sub> Y, HfSb, InLi <sub>2</sub> , As <sub>7</sub> Rb <sub>4</sub> Zn <sub>7</sub> , Li <sub>2</sub> Tl, Hf <sub>3</sub> Sc, NaSi <sub>6</sub> , K <sub>3</sub> O <sub>4</sub> Pd <sub>2</sub> , K <sub>4</sub> P <sub>3</sub> , Ge <sub>4</sub> Li <sub>2</sub> , Pb <sub>2</sub> Y, Ca <sub>4</sub> P <sub>5</sub> Pd <sub>5</sub> , O <sub>4</sub> PTi, PdY, PtScZn, SiY, Sn <sub>2</sub> Y, NbZn <sub>16</sub> , Te <sub>3</sub> Y, PtTaTe <sub>5</sub> , Pd <sub>2</sub> Si <sub>3</sub> Y <sub>3</sub> , Na <sub>9</sub> Sn <sub>4</sub> , Sr <sub>3</sub> Tl <sub>5</sub> , Ge <sub>6</sub> Li <sub>11</sub> , KM <sub>0</sub> <sub>5</sub> O <sub>13</sub> , Ca <sub>7</sub> Li <sub>5</sub> Sn <sub>11</sub> , P <sub>5</sub> Pd <sub>5</sub> Sr <sub>4</sub> , AuTh, AlTh, LuSi, LaPd, LaPt, LaSn, LuSn <sub>2</sub> , Ge <sub>2</sub> Lu, CBU, Ga <sub>2</sub> LuPd, LaMg <sub>2</sub> Pd, In <sub>2</sub> LaPd, Cd <sub>2</sub> LaPd, LaPdSn <sub>2</sub> , BaLaSi <sub>2</sub> , Cd <sub>3</sub> Lu, Ge <sub>2</sub> LaPd, LaZn <sub>4</sub> , S <sub>3</sub> ScU, LaSeTe <sub>2</sub> , LuTe <sub>3</sub> , Ge <sub>2</sub> LaPt, LaTe <sub>3</sub> , LaPtSi <sub>2</sub> , I <sub>3</sub> U, Ge <sub>4</sub> Lu <sub>3</sub> ,

Part 3 of all the predicted **Case 3-TSMs**:

<b>63</b>	Ga <sub>5</sub> U <sub>3</sub> , Th <sub>3</sub> Tl <sub>5</sub> , In <sub>5</sub> Th <sub>3</sub> , La <sub>3</sub> Sn <sub>4</sub> , La <sub>3</sub> Sn <sub>5</sub> , Ge <sub>3</sub> Li <sub>2</sub> Lu <sub>3</sub> , Lu <sub>7</sub> Te, Al <sub>6</sub> Re, Ge <sub>7</sub> Re <sub>3</sub> , B <sub>7</sub> ReY <sub>3</sub> , BrO <sub>2</sub> U, AuCaIn <sub>2</sub> , Ga <sub>5</sub> Zr <sub>3</sub> , N <sub>5</sub> NaTa <sub>3</sub> , K <sub>3</sub> O <sub>4</sub> Pt <sub>2</sub> ,
<b>64</b>	AgCs <sub>2</sub> F <sub>4</sub> , Bi, Au <sub>10</sub> Ca <sub>4</sub> In <sub>3</sub> , Si, NaTl, BCl <sub>14</sub> Zr <sub>6</sub> , CsI <sub>14</sub> Zr <sub>6</sub> , LaSb <sub>2</sub> , Al <sub>3</sub> Ge <sub>4</sub> La <sub>2</sub> , Au <sub>2</sub> Lu <sub>5</sub> Te <sub>2</sub> , I <sub>14</sub> KZr <sub>6</sub> ,
<b>65</b>	Cl <sub>2</sub> Na <sub>3</sub> , B <sub>6</sub> Nb <sub>5</sub> , B <sub>6</sub> Ta <sub>5</sub> , Ga <sub>3</sub> Pt <sub>5</sub> , Ca <sub>7</sub> N <sub>2</sub> Tl <sub>3</sub> , P, B <sub>20</sub> Na <sub>3</sub> , C <sub>3</sub> B <sub>6</sub> Nb <sub>7</sub> , C <sub>2</sub> B <sub>3</sub> Y <sub>2</sub> , O <sub>4</sub> UY, La <sub>3</sub> Sn <sub>7</sub> , Cl <sub>5</sub> O <sub>2</sub> U <sub>2</sub> , Ge <sub>10</sub> La <sub>7</sub> Li <sub>8</sub> , Cs <sub>2</sub> KO <sub>14</sub> Si <sub>4</sub> U <sub>2</sub> , C <sub>7</sub> Re <sub>2</sub> Sc <sub>5</sub> ,
<b>67</b>	Ba <sub>2</sub> NaO,
<b>69</b>	NPd,
<b>70</b>	Au <sub>4</sub> KSn <sub>6</sub> , BPd <sub>6</sub> , C <sub>8</sub> K, C <sub>8</sub> Rb, Nb <sub>3</sub> O <sub>10</sub> U,
<b>71</b>	Y <sub>3</sub> Zn <sub>11</sub> , AgCa <sub>2</sub> Pd <sub>2</sub> , AlSi <sub>2</sub> Y <sub>2</sub> , Au <sub>3</sub> Rb <sub>2</sub> , Br, Ba <sub>3</sub> Hg <sub>10</sub> In, NbPd <sub>2</sub> , NbPt <sub>2</sub> , Hg <sub>11</sub> K <sub>3</sub> , Pd <sub>2</sub> Ta, Br <sub>6</sub> NaO <sub>2</sub> W <sub>2</sub> , In <sub>11</sub> Sr <sub>3</sub> , AlLu <sub>2</sub> Si <sub>2</sub> , KSe <sub>6</sub> U <sub>2</sub> , KSe <sub>6</sub> Th <sub>2</sub> , La <sub>3</sub> Pd <sub>4</sub> Zn <sub>4</sub> , Ge <sub>5</sub> La, La <sub>3</sub> Pd <sub>4</sub> Si <sub>4</sub> , Ge <sub>4</sub> La <sub>3</sub> Pd <sub>4</sub> , Se <sub>6</sub> TlU <sub>2</sub> , Ge <sub>4</sub> La <sub>3</sub> Li <sub>4</sub> , RbSe <sub>6</sub> Th <sub>2</sub> , Ge <sub>16</sub> La <sub>11</sub> Li <sub>12</sub> , ReSi <sub>2</sub> , La <sub>3</sub> Pt <sub>4</sub> Zn <sub>4</sub> , Au <sub>3</sub> K <sub>2</sub> , B <sub>4</sub> Nb <sub>3</sub> , B <sub>4</sub> Ta <sub>3</sub> , Ba <sub>2</sub> Bi <sub>3</sub> , C <sub>4</sub> B <sub>4</sub> Nb <sub>7</sub> ,
<b>74</b>	Au <sub>5</sub> InK <sub>3</sub> , ClNa <sub>2</sub> , Ga <sub>2</sub> Sc, Hg <sub>2</sub> K, Hg <sub>2</sub> Rb, CsHg <sub>2</sub> , P, Si <sub>2</sub> Y, In <sub>2</sub> La, LaZn <sub>2</sub> , LuZn <sub>2</sub> , Ga <sub>2</sub> Lu, LaSi <sub>2</sub> , Au <sub>2</sub> La, Ag <sub>2</sub> La, Ge <sub>2</sub> La, La <sub>3</sub> Pd <sub>5</sub> Si, Au <sub>5</sub> K <sub>3</sub> Tl, Ge <sub>2</sub> NaPd <sub>3</sub> , GaMgMo <sub>4</sub> O <sub>7</sub> ,
<b>75</b>	CNSTI, NbTe <sub>4</sub> ,
<b>79</b>	Sb <sub>2</sub> TlZn <sub>2</sub> , Al <sub>2</sub> Si <sub>3</sub> U <sub>3</sub> ,
<b>83</b>	C <sub>4</sub> UW <sub>4</sub> ,
<b>85</b>	Hf <sub>5</sub> Sb <sub>9</sub> , AgBF <sub>5</sub> , Se <sub>3</sub> Tl <sub>5</sub> ,
<b>86</b>	Nb <sub>3</sub> P, GeHf <sub>3</sub> , Hf <sub>3</sub> P, AsNb <sub>3</sub> , AsTi <sub>3</sub> , GeZr <sub>3</sub> , PTi <sub>3</sub> , SiZr <sub>3</sub> , SiTi <sub>3</sub> , AsTa <sub>3</sub> , PTa <sub>3</sub> , GeLa <sub>3</sub> ,
<b>87</b>	Au <sub>4</sub> Sc, Hg <sub>19</sub> Rb <sub>5</sub> , Ag <sub>4</sub> Sc, N <sub>5</sub> Nb <sub>4</sub> , Nb <sub>5</sub> Se <sub>4</sub> , Nb <sub>5</sub> Te <sub>4</sub> , Nb <sub>5</sub> Sb <sub>4</sub> , As <sub>4</sub> Ta <sub>5</sub> , Sb <sub>4</sub> Ta <sub>5</sub> , As <sub>4</sub> Nb <sub>5</sub> Pd <sub>4</sub> , Nb <sub>5</sub> P <sub>4</sub> Pd <sub>4</sub> , Ba <sub>9</sub> In <sub>4</sub> , Pt <sub>11</sub> Zr <sub>9</sub> , Pt <sub>12</sub> Si <sub>5</sub> , In <sub>4</sub> Pd <sub>17</sub> Se <sub>4</sub> , S <sub>8</sub> Zr <sub>21</sub> , Nb <sub>21</sub> S <sub>8</sub> , Cs <sub>5</sub> Hg <sub>19</sub> , Cs <sub>3</sub> Te <sub>22</sub> , Au <sub>4</sub> Lu, F <sub>5</sub> U, O <sub>6</sub> ReSr <sub>2</sub> Zn, Ba <sub>2</sub> CaO <sub>6</sub> Re,
<b>88</b>	CsFO <sub>3</sub> S, GaMg, O <sub>4</sub> Pd <sub>2</sub> Y, Ge <sub>8</sub> Pd <sub>21</sub> , Al <sub>21</sub> Pd <sub>8</sub> , Al <sub>17</sub> Pd <sub>8</sub> Si <sub>4</sub> , Al <sub>21</sub> Pt <sub>8</sub> , LaO <sub>4</sub> Pd <sub>2</sub> ,
<b>92</b>	MgO <sub>4</sub> Ti <sub>2</sub> , Si <sub>4</sub> Ti <sub>5</sub> , Hf <sub>2</sub> Sc <sub>3</sub> Si <sub>4</sub> , Pr <sub>5</sub> Si <sub>4</sub> , Re <sub>3</sub> Sc <sub>2</sub> Si <sub>4</sub> ,
<b>95</b>	LiNbO <sub>4</sub> Zn,
<b>97</b>	ISe <sub>8</sub> Ta <sub>2</sub> ,
<b>102</b>	U,
<b>103</b>	TaTe <sub>4</sub> , NbTe <sub>4</sub> , NbSe <sub>4</sub> ,
<b>104</b>	Ba <sub>5</sub> Bi <sub>5</sub> In <sub>4</sub> ,
<b>107</b>	GeP, PSn, LiPdSi <sub>3</sub> , In <sub>2</sub> Te <sub>3</sub> , AsGe, AuSi <sub>3</sub> Sr, AuBaSn <sub>3</sub> , BaGe <sub>3</sub> Pd, Al <sub>3</sub> AuLa,

Part 4 of all the predicted **Case 3-TSMs**:

<b>108</b>	Bi <sub>2</sub> O <sub>4</sub> Pd, Ca <sub>5</sub> Ge <sub>3</sub> , K <sub>2</sub> Se <sub>4</sub> Sn <sub>2</sub> ,
<b>109</b>	AsCaPt, LiMo <sub>8</sub> O <sub>10</sub> , GeLaPt,
<b>110</b>	As <sub>2</sub> Cd <sub>3</sub> ,
<b>113</b>	NaSn <sub>5</sub> , Ta <sub>22</sub> , Ta <sub>30</sub> , Ta,
<b>115</b>	CB <sub>2</sub> N, PdSb <sub>3</sub> Zr <sub>2</sub> , C <sub>7</sub> B, Hf <sub>2</sub> PdSb <sub>3</sub> ,
<b>120</b>	Au <sub>4</sub> KSn <sub>2</sub> ,
<b>121</b>	Au <sub>12</sub> K <sub>23</sub> Sn <sub>9</sub> ,
<b>123</b>	AgTi, PtZn, CdPt <sub>2</sub> Zn, AsHgPd <sub>5</sub> , AsGaPd <sub>5</sub> , GaPPd <sub>5</sub> , AsPt <sub>5</sub> Zn, CdPPt <sub>5</sub> , BaBi <sub>2</sub> OTi <sub>2</sub> , In <sub>2</sub> Pd <sub>8</sub> Se, BaNb <sub>4</sub> O <sub>6</sub> , BaNb <sub>7</sub> O <sub>9</sub> , AlTi, AlPt <sub>3</sub> , AgZr <sub>3</sub> , AgHg <sub>2</sub> Ti, AsCdPd <sub>5</sub> , CaPb, CdPd, CdPt, InMg, Au <sub>3</sub> Cd, PdT <sub>i</sub> , SnTl, HgPd, GaTi, HgPt, SiSr, Cd <sub>3</sub> Zr, Hg <sub>2</sub> Pt, Pd <sub>3</sub> Tl, InPd <sub>3</sub> , BaBi <sub>3</sub> , As <sub>2</sub> BaPd <sub>2</sub> , Sr, BaP <sub>2</sub> Pd <sub>2</sub> , InPt <sub>3</sub> , AsInPd <sub>5</sub> , AuCl <sub>3</sub> Cs, AsPd <sub>5</sub> Tl, AlPPt <sub>5</sub> , HgPd <sub>5</sub> Se, CdPd <sub>5</sub> Se, MgPPd <sub>5</sub> , InPd <sub>5</sub> Se, CdPPd <sub>5</sub> , Pd <sub>5</sub> SeZn, HgPPd <sub>5</sub> , InPPd <sub>5</sub> , AsMgPt <sub>5</sub> , CGaPt <sub>3</sub> , AsCdPt <sub>5</sub> , PPd <sub>5</sub> Zn, AgPPt <sub>5</sub> , PPd <sub>5</sub> Tl, PPd <sub>5</sub> Sn, AsPt <sub>5</sub> Tl, AgPt <sub>5</sub> Si, Pt <sub>5</sub> SbSi, MgPPt <sub>5</sub> , PPt <sub>5</sub> Zn, InPPt <sub>5</sub> , PbPt <sub>5</sub> Si, Pt <sub>5</sub> SiTl, FKNb <sub>4</sub> O <sub>5</sub> , InPt <sub>5</sub> Si, PPt <sub>5</sub> Tl, PPt <sub>5</sub> Sn, AsIn <sub>2</sub> Pt <sub>8</sub> , Nb <sub>5</sub> O <sub>9</sub> Sr <sub>2</sub> , KO <sub>5</sub> S <sub>2</sub> Ti <sub>2</sub> Y <sub>2</sub> , Ba <sub>2</sub> Nb <sub>5</sub> O <sub>9</sub> , Nb <sub>4</sub> O <sub>6</sub> Sr, AsLa, AgLa, CdLa, LaSb, Ga <sub>5</sub> PdU, Ga <sub>6</sub> LaPd, Ga <sub>5</sub> PtU, C <sub>2</sub> Re,
<b>124</b>	NbTe <sub>4</sub> , TaTe <sub>4</sub> ,
<b>125</b>	Ga <sub>6</sub> Y, Ag <sub>5</sub> RbSe <sub>3</sub> , Ga <sub>6</sub> La,
<b>126</b>	Cd <sub>32</sub> K <sub>6</sub> ,
<b>127</b>	Hg <sub>5</sub> Pd <sub>2</sub> , Hf <sub>2</sub> In <sub>5</sub> , Be <sub>2</sub> Nb <sub>3</sub> , AlSc <sub>2</sub> Si <sub>2</sub> , Au <sub>2</sub> Ca <sub>2</sub> Pb, PbPd <sub>2</sub> Y <sub>2</sub> , InPd <sub>2</sub> Y <sub>2</sub> , LiSi <sub>2</sub> Y <sub>2</sub> , B <sub>2</sub> Nb <sub>3</sub> , B <sub>2</sub> Mo <sub>3</sub> , Ga <sub>2</sub> Nb <sub>3</sub> , Ga <sub>2</sub> MgSc <sub>2</sub> , Ca <sub>3</sub> Hg <sub>2</sub> , Be <sub>2</sub> Ta <sub>3</sub> , B <sub>2</sub> Mo <sub>2</sub> Nb, Au <sub>2</sub> InY <sub>2</sub> , B <sub>2</sub> Mo <sub>2</sub> Ta, B <sub>2</sub> Ta <sub>3</sub> , C <sub>2</sub> B <sub>2</sub> Y, In <sub>5</sub> Ti <sub>2</sub> , Ga <sub>5</sub> W <sub>2</sub> , Hg <sub>2</sub> Sr <sub>3</sub> , Ge <sub>2</sub> Hf <sub>3</sub> , Ga <sub>2</sub> Ta <sub>3</sub> , Mo <sub>3</sub> Si <sub>2</sub> , Nb <sub>3</sub> Si <sub>2</sub> , Si <sub>2</sub> W <sub>3</sub> , LiPd <sub>2</sub> Sn <sub>6</sub> , KMo <sub>4</sub> O <sub>6</sub> , Mo <sub>4</sub> NaO <sub>6</sub> , Mo <sub>4</sub> O <sub>6</sub> Sn, B <sub>4</sub> W, InPd <sub>2</sub> Th <sub>2</sub> , C <sub>2</sub> B <sub>2</sub> La, B <sub>4</sub> Th, InLa <sub>2</sub> Pd <sub>2</sub> , InPd <sub>2</sub> U <sub>2</sub> , Ge <sub>2</sub> InLa <sub>2</sub> , InLu <sub>2</sub> Pd <sub>2</sub> , C <sub>2</sub> B <sub>2</sub> Lu, Ge <sub>2</sub> Lu <sub>2</sub> Mg, La <sub>2</sub> PbPd <sub>2</sub> , InPt <sub>2</sub> U <sub>2</sub> , La <sub>3</sub> Si <sub>2</sub> , N <sub>2</sub> Re, O <sub>3</sub> Re, B <sub>2</sub> ReTi <sub>2</sub> , ClF <sub>6</sub> K <sub>3</sub> Re, Pd <sub>2</sub> SnU <sub>2</sub> , Lu <sub>2</sub> PbPd <sub>2</sub> , Pt <sub>2</sub> SnU <sub>2</sub> , Ba <sub>3</sub> O <sub>15</sub> Ta <sub>5</sub> , Al <sub>2</sub> Th <sub>3</sub> , Ga <sub>2</sub> Th <sub>3</sub> , Ge <sub>2</sub> Th <sub>3</sub> ,
<b>128</b>	Cl <sub>6</sub> K <sub>2</sub> Nb, F <sub>14</sub> K <sub>5</sub> Ti <sub>3</sub> , Re <sub>3</sub> Si <sub>5</sub> Y <sub>2</sub> , Pd <sub>4</sub> Rb <sub>2</sub> Se <sub>17</sub> U <sub>6</sub> ,
<b>129</b>	AuHf, BBe <sub>4</sub> , PSnSr, AuTi, AgZr, AsNbSi, AgTi, SiTiY, PdT <sub>a</sub> , BiIn, AgHf, S <sub>2</sub> Y, GeTiY, AsSiTa, GeTeZr, SbSc <sub>2</sub> , MoNTa, GeSbTi, GeSbZr, AgMgSb, NbSbSi, BaMgSi, Te <sub>2</sub> Y, BiKMg, Sn <sub>2</sub> YZn, Au <sub>2</sub> BaSn <sub>2</sub> , As <sub>2</sub> Pt <sub>2</sub> Sr, Au <sub>3</sub> BaGe, Au <sub>3</sub> GeSr, Pt <sub>2</sub> Si <sub>2</sub> Y, Au <sub>3</sub> BaSi, Bi <sub>9</sub> Ti <sub>8</sub> , AsSeTh, Al <sub>2</sub> Au <sub>2</sub> U, GeLaTi, AsSU, BiSbU, AsSbU, BiTeTh, BiTeU, LaS <sub>2</sub> , AsSeU, As <sub>2</sub> Pa, LuS <sub>2</sub> , Al <sub>2</sub> LaPd <sub>2</sub> , LaPdSb <sub>2</sub> , Ga <sub>2</sub> LaPd <sub>2</sub> , LaTe <sub>2</sub> , AsTeTh, P <sub>2</sub> Pa, Al <sub>2</sub> Au <sub>2</sub> La, NTeU, PaSb <sub>2</sub> , BiLa <sub>2</sub> N, SbTeTh, PSeU, PSeTh, GeLuTi, Bi <sub>2</sub> Th, As <sub>2</sub> Th, PSU, PSTh, LuSe <sub>2</sub> , Bi <sub>2</sub> U, SSbU, AuSb <sub>2</sub> U,

Part 5 of all the predicted **Case 3-TSMs**:

129	LuTe <sub>2</sub> , SbSeU, LuSiTi, LaPd <sub>2</sub> Sb <sub>2</sub> , LaSe <sub>2</sub> , SbSeTh, Sb <sub>2</sub> Th, AuBi <sub>2</sub> La, LuSn <sub>2</sub> Zn, Te <sub>2</sub> U, SbTeU, Au <sub>2</sub> Si <sub>2</sub> U, Ge <sub>2</sub> LaPt <sub>2</sub> , Pt <sub>2</sub> Si <sub>2</sub> U, LaPt <sub>2</sub> Si <sub>2</sub> , AsSTh, AsTeU,
130	AlMg <sub>4</sub> Si <sub>3</sub> , Se <sub>3</sub> Tl <sub>5</sub> , AuBi <sub>2</sub> O <sub>5</sub> , Ge <sub>3</sub> La <sub>5</sub> ,
131	OPd, NPd, C <sub>2</sub> B <sub>2</sub> Lu, C <sub>2</sub> B <sub>2</sub> La,
132	O <sub>2</sub> Si, Bi <sub>2</sub> O <sub>3</sub> ,
134	B, Ag <sub>2</sub> Li <sub>3</sub> Si <sub>3</sub> , Ag <sub>2</sub> Ge <sub>3</sub> Li <sub>3</sub> , B,
135	CB <sub>2</sub> Y,
136	InPd <sub>2</sub> Sc <sub>2</sub> , BiPb <sub>3</sub> Pt, Ta, O <sub>2</sub> Pd, NbO <sub>2</sub> , NTi <sub>2</sub> , O <sub>2</sub> Pt, Au <sub>2</sub> InSc <sub>2</sub> , Au <sub>2</sub> Sc <sub>2</sub> Sn, Au <sub>2</sub> InZr <sub>2</sub> , InPd <sub>2</sub> Zr <sub>2</sub> , F <sub>6</sub> Na <sub>2</sub> Nb, Au <sub>2</sub> Hf <sub>2</sub> In, Hf <sub>2</sub> InPd <sub>2</sub> , Au <sub>2</sub> SnY <sub>2</sub> , Au <sub>2</sub> SnY <sub>2</sub> , AuTa <sub>2</sub> , Al <sub>2</sub> Pt <sub>4</sub> Ti <sub>9</sub> , AlTa <sub>2</sub> , Ca <sub>11</sub> N <sub>8</sub> , Ga <sub>6</sub> Na <sub>10</sub> Sn <sub>3</sub> , InPt <sub>2</sub> U <sub>2</sub> , Au <sub>2</sub> Lu <sub>2</sub> Sn, Au <sub>2</sub> InLu <sub>2</sub> , Pt <sub>2</sub> SnU <sub>2</sub> , U, O <sub>2</sub> Re, Re <sub>4</sub> Si <sub>2</sub> Y, AlNb <sub>2</sub> , Bi <sub>2</sub> MgO <sub>6</sub> , O <sub>2</sub> Pb,
137	Bi <sub>2</sub> Se <sub>3</sub> , Cd <sub>3</sub> P <sub>2</sub> , TeTl, As <sub>2</sub> Cd <sub>3</sub> , B <sub>4</sub> Re <sub>4</sub> Y, Nb <sub>4</sub> O <sub>5</sub> ,
139	AlAu <sub>2</sub> , Au <sub>2</sub> Ti, AuZr <sub>2</sub> , MoSi <sub>2</sub> , GeSb, Ge <sub>2</sub> W, Al <sub>4</sub> Ca, BaGa <sub>4</sub> , Al <sub>4</sub> Sr, Ga <sub>4</sub> Sr, Be <sub>12</sub> Ti, B <sub>12</sub> Sc, AlI <sub>2</sub> Pd <sub>5</sub> , AgCs <sub>2</sub> F <sub>4</sub> , Na <sub>2</sub> OSb <sub>2</sub> Ti <sub>2</sub> , CaGe <sub>3</sub> , AuORb, Cl <sub>10</sub> K <sub>4</sub> OW <sub>2</sub> , Ag <sub>2</sub> Sc, Ag <sub>2</sub> Y, AgHf <sub>2</sub> , Al <sub>2</sub> BaSi <sub>2</sub> , Ag <sub>2</sub> Si <sub>2</sub> Sr, Ag <sub>2</sub> Sn <sub>2</sub> Sr, Ag <sub>2</sub> Ge <sub>2</sub> Sr, Al <sub>2</sub> Pb <sub>2</sub> Sr, Al <sub>3</sub> Nb, Al <sub>3</sub> Ti, Al <sub>3</sub> Ta, AgBe <sub>12</sub> , Br, In <sub>4</sub> Sr, AuHf <sub>2</sub> , Au <sub>2</sub> Nb <sub>3</sub> , CdTi <sub>2</sub> , Al <sub>4</sub> Ba, Bi, Au <sub>2</sub> Sc, Ga <sub>3</sub> Ta, Au <sub>2</sub> Y, CaGa <sub>4</sub> , Ga, Ga <sub>3</sub> Nb, Sc, Tl, P <sub>2</sub> Pd <sub>2</sub> Y, Be <sub>12</sub> Pd, OPd, AuBe <sub>12</sub> , Au <sub>2</sub> Si <sub>2</sub> Y, BaIn <sub>4</sub> , Ga <sub>4</sub> Na, Cl <sub>2</sub> O <sub>4</sub> Pb <sub>4</sub> , Al <sub>3</sub> Zr, In, AgTi <sub>2</sub> , BiO <sub>2</sub> Y <sub>2</sub> , Hf <sub>2</sub> Tl, Sb, Ga <sub>3</sub> Ti, I, NbPd <sub>3</sub> , S <sub>2</sub> Ti, NbS <sub>2</sub> , C <sub>2</sub> Y, Pd <sub>3</sub> Tl, Be <sub>12</sub> Ta, Au <sub>4</sub> CaCd <sub>2</sub> , Ge <sub>2</sub> Mo, Si <sub>2</sub> W, Pd <sub>2</sub> Si <sub>2</sub> Y, Ga <sub>3</sub> Hf, Pd <sub>3</sub> Ta, Al <sub>2</sub> Pd <sub>5</sub> Y, Ge <sub>2</sub> Pd <sub>2</sub> Sr, Be <sub>12</sub> Pt, N <sub>3</sub> Nb <sub>4</sub> , Pt <sub>2</sub> Si, Rb, Pt <sub>2</sub> Si <sub>2</sub> Y, F <sub>4</sub> Nb, Be <sub>12</sub> Nb, C <sub>2</sub> BSc <sub>2</sub> , GeTiY, Ga <sub>4</sub> Ti <sub>2</sub> Y, KO <sub>2</sub> , In <sub>4</sub> K, C <sub>2</sub> Bi <sub>2</sub> CaO <sub>8</sub> , N <sub>2</sub> Sr, As <sub>2</sub> BaPd <sub>2</sub> , Pt <sub>3</sub> Sb, Ag <sub>2</sub> CaGe <sub>2</sub> , YZn <sub>12</sub> , ScZn <sub>12</sub> , Ga <sub>5</sub> Mg <sub>2</sub> , Cl <sub>6</sub> NbRb <sub>2</sub> , Ge <sub>3</sub> Sr, BaBi <sub>4</sub> Cl <sub>2</sub> O <sub>6</sub> , Ca <sub>2</sub> Na <sub>2</sub> O <sub>10</sub> Ta <sub>3</sub> , Ge <sub>4</sub> In <sub>6</sub> Y <sub>11</sub> , Ge <sub>10</sub> Sc <sub>11</sub> , Sn <sub>10</sub> Y <sub>11</sub> , In <sub>6</sub> Si <sub>4</sub> Y <sub>11</sub> , Ca <sub>11</sub> Sb <sub>10</sub> , Sb <sub>10</sub> Sr <sub>11</sub> , Ag <sub>2</sub> Lu, Al <sub>2</sub> LaZn <sub>2</sub> , Au <sub>2</sub> Lu, Au <sub>2</sub> Si <sub>2</sub> Th, Au <sub>2</sub> Ge <sub>2</sub> Th, BiLa <sub>2</sub> , Al <sub>4</sub> La, BiN <sub>2</sub> U <sub>2</sub> , Al <sub>2</sub> Ga <sub>2</sub> La, As <sub>2</sub> LaPd <sub>2</sub> , Au <sub>2</sub> LaSi <sub>2</sub> , Ag <sub>2</sub> LaSi <sub>2</sub> , C <sub>2</sub> Lu, Ge <sub>2</sub> Pd <sub>2</sub> U, BiLa <sub>2</sub> O <sub>2</sub> , C <sub>2</sub> Pa, La, AsTeU, I <sub>2</sub> La, Pa, Li <sub>3</sub> O <sub>4</sub> U, Ge <sub>2</sub> LaPd <sub>2</sub> , LaP <sub>2</sub> Pd <sub>2</sub> , MoU <sub>2</sub> , BiN <sub>2</sub> Th <sub>2</sub> , Ge <sub>2</sub> LaPt <sub>2</sub> , LuPb <sub>2</sub> , LaPd <sub>2</sub> Si <sub>2</sub> , Ga <sub>4</sub> LuTi <sub>2</sub> , LuPd <sub>2</sub> Si <sub>2</sub> , GeTeTh, Pd <sub>2</sub> Si <sub>2</sub> U, GeSeTh, LuPt <sub>2</sub> Si <sub>2</sub> , N <sub>2</sub> SbU <sub>2</sub> , N <sub>2</sub> TeU <sub>2</sub> , CB <sub>2</sub> Pt <sub>2</sub> Th, N <sub>2</sub> SbTh <sub>2</sub> , SiTeTh, La <sub>3</sub> N <sub>6</sub> Ta <sub>2</sub> , O <sub>4</sub> Sr <sub>2</sub> U, LaMg <sub>12</sub> , LuO <sub>4</sub> S <sub>5</sub> U <sub>4</sub> , LuZn <sub>12</sub> , LaLi <sub>2</sub> O <sub>7</sub> Ta <sub>2</sub> , LuSi <sub>3</sub> , La <sub>3</sub> N <sub>6</sub> Nb <sub>2</sub> , Ge <sub>10</sub> Lu <sub>11</sub> , AlRe <sub>2</sub> , C <sub>2</sub> Re, ReSi <sub>2</sub> , Cl <sub>10</sub> Cs <sub>3</sub> ORe <sub>2</sub> , ZnZr <sub>2</sub> ,
140	Pb <sub>2</sub> Pd, AuPb <sub>2</sub> , AlHf <sub>2</sub> , Ga <sub>2</sub> SnTa <sub>5</sub> , GaNb <sub>5</sub> Sn <sub>2</sub> , Mo <sub>5</sub> Si <sub>3</sub> , Nb <sub>20</sub> Si <sub>12</sub> , Si <sub>3</sub> Ta <sub>5</sub> , In <sub>3</sub> Sr <sub>5</sub> , FPb <sub>3</sub> Sr <sub>5</sub> , AlZr <sub>2</sub> , BMo <sub>2</sub> , Sr, AgIn <sub>2</sub> , AuNa <sub>2</sub> , SZr <sub>2</sub> , Ba, BTi <sub>2</sub> , GaHf <sub>2</sub> , GeHf <sub>2</sub> , PdTl <sub>2</sub> , AuTl <sub>2</sub> , BW <sub>2</sub> , GaZr <sub>2</sub> , BTa <sub>2</sub> , GaPt <sub>3</sub> , AgF <sub>3</sub> Rb, Ga <sub>5</sub> Pd, AgCsF <sub>3</sub> , Al <sub>3</sub> Zr <sub>5</sub> , Au <sub>4</sub> In <sub>2</sub> Rb, Au <sub>4</sub> In <sub>2</sub> K, Nb <sub>5</sub> Si <sub>3</sub> , Ge <sub>3</sub> Nb <sub>5</sub> , BGe <sub>2</sub> Nb <sub>5</sub> , Ge <sub>3</sub> Mo <sub>5</sub> , Ga <sub>3</sub> Nb <sub>5</sub> , Ga <sub>3</sub> NbZr <sub>4</sub> , Nb <sub>5</sub> SiSn <sub>2</sub> , Ga <sub>3</sub> Ti <sub>5</sub> , Au <sub>3</sub> Cd <sub>5</sub> , Ge <sub>3</sub> W <sub>5</sub> , Au <sub>3</sub> Ca <sub>5</sub> , Ge <sub>3</sub> Ta <sub>5</sub> , W <sub>5</sub> Zr <sub>3</sub> , Bi <sub>3</sub> In <sub>4</sub> Pb, AuSe <sub>3</sub> Tl <sub>4</sub> , Ca <sub>5</sub> Ga <sub>3</sub> , Ag <sub>3</sub> Ca <sub>5</sub> , Ca <sub>5</sub> Ge <sub>3</sub> , Ca <sub>5</sub> Si <sub>3</sub> , Ca <sub>5</sub> Zn <sub>3</sub> , Ca <sub>5</sub> Pt <sub>3</sub> , Pb <sub>3</sub> Sr <sub>5</sub> , B <sub>2</sub> GeTa <sub>5</sub> ,

Part 6 of all the predicted **Case 3-TSMs**:

140	Te <sub>3</sub> Tl <sub>5</sub> , TeTl, Si <sub>3</sub> W <sub>5</sub> , Sr <sub>5</sub> Tl <sub>3</sub> , Ba <sub>5</sub> Pb <sub>3</sub> , Ba <sub>11</sub> In <sub>6</sub> O <sub>3</sub> , GeTh <sub>2</sub> , InTh <sub>2</sub> , AuTh <sub>2</sub> , AlTh <sub>2</sub> , PdTh <sub>2</sub> , Th <sub>2</sub> Zn, GaTh <sub>2</sub> , AgTh <sub>2</sub> , HgTh <sub>2</sub> , Th <sub>2</sub> Tl, ClGa <sub>4</sub> La <sub>3</sub> , Ge <sub>2</sub> La <sub>5</sub> Si, S <sub>5</sub> U <sub>3</sub> , La <sub>5</sub> Si <sub>3</sub> , Lu <sub>5</sub> Pd <sub>2</sub> Sb, Ga <sub>3</sub> La <sub>5</sub> , La <sub>5</sub> SnZn <sub>2</sub> , La <sub>5</sub> Sn <sub>3</sub> , AuF <sub>11</sub> U <sub>2</sub> , Cl <sub>4</sub> Ga <sub>5</sub> La <sub>10</sub> , Br <sub>4</sub> Ga <sub>5</sub> La <sub>10</sub> , Al <sub>5</sub> Br <sub>4</sub> La <sub>10</sub> , Re <sub>5</sub> Si <sub>3</sub> , Al <sub>4</sub> Br <sub>4</sub> La <sub>5</sub> , La <sub>5</sub> Tl <sub>3</sub> , BeTa <sub>2</sub> , Cs <sub>9</sub> InO <sub>4</sub> ,
141	K, Cs, Mo <sub>2</sub> N, Ge <sub>2</sub> Y, LiSn, In <sub>2</sub> NSr <sub>4</sub> , AuLi <sub>2</sub> Sn <sub>2</sub> , Ca <sub>4</sub> In <sub>2</sub> N, O <sub>5</sub> Ta <sub>2</sub> , CCl <sub>13</sub> Cs <sub>4</sub> Sc <sub>6</sub> , Rb, Sr, Si <sub>2</sub> Y, LiO <sub>2</sub> Ti, NTi <sub>2</sub> , GeLi, AgLi <sub>2</sub> Sn <sub>2</sub> , LaSi <sub>2</sub> , PbTh, LiN <sub>2</sub> U, Cl <sub>4</sub> U, Ge <sub>2</sub> La, LaMgSi <sub>2</sub> , Cl <sub>4</sub> Pa, Br <sub>4</sub> Pa, O <sub>4</sub> SiU, LaZn <sub>11</sub> , La <sub>3</sub> Zn <sub>22</sub> , B <sub>4</sub> Re <sub>4</sub> , Ag <sub>6</sub> GeO <sub>8</sub> S,
142	Pd <sub>16</sub> Sn <sub>32</sub> , PdSn <sub>2</sub> ,
143	BiTe, AlCaSi,
146	CBr <sub>12</sub> Sc <sub>7</sub> , Au <sub>5</sub> Sn, P <sub>3</sub> Pd <sub>7</sub> , CI <sub>12</sub> Sc <sub>7</sub> , Cl <sub>6</sub> LiW,
147	Cl <sub>18</sub> Cs <sub>2</sub> W <sub>6</sub> , NW <sub>2</sub> , Au <sub>10</sub> In <sub>3</sub> , Br <sub>2</sub> Hg <sub>3</sub> Se <sub>3</sub> Zn,
148	F <sub>6</sub> PdPt, CsMo <sub>6</sub> Se <sub>7</sub> , Cl <sub>12</sub> Zr <sub>6</sub> , BCl <sub>12</sub> Sc <sub>7</sub> , Cl <sub>3</sub> Ti, F <sub>6</sub> PdZr, F <sub>6</sub> LiPt, Br <sub>3</sub> Ti, AgBiO <sub>3</sub> , Pd <sub>4</sub> Zr <sub>3</sub> , Au <sub>4</sub> Ca <sub>3</sub> , Mo <sub>6</sub> Te <sub>8</sub> , Mo <sub>6</sub> Se <sub>8</sub> Y, HgMo <sub>6</sub> S <sub>8</sub> , CaMo <sub>6</sub> S <sub>8</sub> , Ca <sub>3</sub> Pd <sub>2</sub> , AgMo <sub>6</sub> Se <sub>8</sub> , Mo <sub>6</sub> S <sub>8</sub> Y, BiMo <sub>6</sub> S <sub>8</sub> , InMo <sub>6</sub> Se <sub>8</sub> , BaMo <sub>6</sub> S <sub>8</sub> , AgMo <sub>6</sub> S <sub>8</sub> , KO <sub>3</sub> Sb, Mo <sub>6</sub> NbS <sub>8</sub> , Mo <sub>6</sub> PbS <sub>8</sub> , InMo <sub>6</sub> S <sub>8</sub> , Mo <sub>6</sub> S <sub>8</sub> Sr, Mo <sub>6</sub> S <sub>8</sub> Sn, Ca <sub>3</sub> Pt <sub>2</sub> , LiMo <sub>6</sub> Se <sub>8</sub> , Mo <sub>6</sub> S <sub>8</sub> Sb, Cl <sub>12</sub> Sc <sub>7</sub> , Mo <sub>6</sub> Se <sub>8</sub> Tl, Mo <sub>6</sub> Se <sub>8</sub> Sn, Mo <sub>6</sub> PbSe <sub>8</sub> , Mo <sub>6</sub> S <sub>8</sub> Tl, Pt <sub>2</sub> Sr <sub>3</sub> , Ag <sub>2</sub> Sr <sub>3</sub> , Au <sub>2</sub> Ba <sub>3</sub> , AlPd, Br <sub>12</sub> Zr <sub>6</sub> , Pd <sub>4</sub> Y <sub>3</sub> , Pd <sub>2</sub> Y <sub>3</sub> , I <sub>12</sub> Zr <sub>6</sub> , P <sub>2</sub> Pd <sub>15</sub> , Pd <sub>20</sub> Sb <sub>7</sub> , Pd <sub>20</sub> Te <sub>7</sub> , NaO <sub>13</sub> Ti <sub>8</sub> , Cl <sub>18</sub> W <sub>6</sub> , Mo <sub>12</sub> Rb <sub>2</sub> Se <sub>14</sub> , Cl <sub>18</sub> K <sub>2</sub> Zr <sub>7</sub> , BI <sub>12</sub> Zr <sub>6</sub> , Cs <sub>2</sub> Mo <sub>12</sub> Se <sub>14</sub> , Mo <sub>18</sub> Rb <sub>4</sub> Se <sub>20</sub> , CsF <sub>6</sub> U, I <sub>6</sub> Na <sub>2</sub> U, Lu <sub>3</sub> Pd <sub>4</sub> , LuMo <sub>6</sub> S <sub>8</sub> , La <sub>3</sub> Pd <sub>4</sub> , Mo <sub>6</sub> S <sub>8</sub> U, LuMo <sub>6</sub> Se <sub>8</sub> , Pd <sub>4</sub> Th <sub>3</sub> , LaMo <sub>6</sub> S <sub>8</sub> , Lu <sub>3</sub> Pt <sub>4</sub> , La <sub>3</sub> Pt <sub>4</sub> , LaMo <sub>6</sub> Se <sub>8</sub> , Cl <sub>18</sub> LuNb <sub>6</sub> , CCl <sub>18</sub> Cs <sub>2</sub> Lu <sub>7</sub> , Ga <sub>40</sub> LaMo <sub>8</sub> , Cl <sub>6</sub> Re, Ag <sub>2</sub> Cl <sub>6</sub> Re, CsF <sub>6</sub> Re, O <sub>12</sub> ReSc <sub>6</sub> , Ba <sub>6</sub> N <sub>6</sub> ORe <sub>2</sub> , P <sub>13</sub> Re <sub>6</sub> , P <sub>26</sub> Re <sub>12</sub> , Cl <sub>12</sub> ReTe <sub>2</sub> , Br <sub>2</sub> Mo <sub>6</sub> S <sub>6</sub> , Ag <sub>2</sub> Ba <sub>3</sub> , Au <sub>2</sub> Sr <sub>3</sub> , Cs <sub>2</sub> Mo <sub>12</sub> Te <sub>14</sub> , I <sub>6</sub> MoO <sub>18</sub> Rb <sub>2</sub> ,
149	Cl <sub>3</sub> Ti,
150	F <sub>3</sub> Pd,
152	Te,
154	HgSe,
155	OZr <sub>3</sub> , Li <sub>4</sub> Pt <sub>3</sub> Si, HgMg <sub>3</sub> , Ag <sub>3</sub> BO <sub>3</sub> ,
156	CB <sub>2</sub> N, C <sub>7</sub> B, CdS <sub>2</sub> Tl, CaLiSn, Cl <sub>6</sub> K <sub>2</sub> NaU,
157	Ag <sub>5</sub> O <sub>6</sub> Pb <sub>2</sub> , AuCd, Al <sub>40</sub> Ba <sub>21</sub> , CsNO <sub>3</sub> ,
158	Cl <sub>15</sub> HgS <sub>3</sub> Se <sub>3</sub> Zn,
159	C <sub>5</sub> Al <sub>3</sub> Zr <sub>2</sub> , C <sub>5</sub> Al <sub>3</sub> Hf <sub>2</sub> ,
160	AsSe <sub>2</sub> , AgTe <sub>3</sub> , BiO, CB <sub>2</sub> N, As <sub>3</sub> Sn <sub>4</sub> , HgS <sub>2</sub> Ta, B <sub>4</sub> Li <sub>5</sub> , Br <sub>2</sub> Ca <sub>3</sub> Si, KS <sub>2</sub> Sn, NbSe <sub>2</sub> , KS <sub>2</sub> Ti, In <sub>2</sub> S <sub>4</sub> Zn, AlMo <sub>4</sub> S <sub>8</sub> , C <sub>3</sub> Al <sub>8</sub> N <sub>4</sub> , GaMo <sub>4</sub> S <sub>8</sub> , GaMo <sub>4</sub> Se <sub>8</sub> , C <sub>7</sub> B, Cs <sub>2</sub> O <sub>12</sub> U <sub>4</sub> ,
161	Ge <sub>3</sub> Li <sub>8</sub> Zn <sub>2</sub> , Ge <sub>13</sub> Pt <sub>4</sub> Y <sub>3</sub> , LiO <sub>3</sub> U, LiO <sub>3</sub> Re, Li <sub>2</sub> O <sub>3</sub> Re,

Part 7 of all the predicted **Case 3-TSMs**:

<b>162</b>	F <sub>6</sub> Li <sub>2</sub> Nb, NNb <sub>2</sub> , As <sub>2</sub> O <sub>6</sub> Pd, NTa <sub>2</sub> , F <sub>6</sub> Hg <sub>3</sub> Nb, CW <sub>2</sub> , Ag <sub>5</sub> O <sub>6</sub> Pb <sub>2</sub> , MoN, AgSe <sub>2</sub> Tl,
<b>163</b>	OTi <sub>3</sub> , Cl <sub>3</sub> Ti, In <sub>2</sub> Pt <sub>3</sub> , F <sub>6</sub> GaLiPd, AlF <sub>6</sub> LiPd, Cl <sub>6</sub> MoNa <sub>3</sub> , KM <sub>0</sub> <sub>12</sub> S <sub>14</sub> , Cl <sub>18</sub> CsPbTa <sub>6</sub> ,
<b>164</b>	NbS <sub>2</sub> , O <sub>2</sub> PZr <sub>3</sub> , CdInS <sub>2</sub> , Ag <sub>2</sub> F, Cl <sub>2</sub> Ti, AuTe <sub>2</sub> , AlCl <sub>3</sub> , CaHg <sub>2</sub> , CSc <sub>2</sub> , Cd <sub>2</sub> Y, CdSe <sub>2</sub> Tl, CdTe <sub>2</sub> Tl, Cl <sub>2</sub> NSc <sub>2</sub> , Au <sub>3</sub> In <sub>2</sub> , Al <sub>2</sub> Ge <sub>2</sub> Y, CdS <sub>2</sub> Tl, CaSb <sub>2</sub> Zn <sub>2</sub> , Al <sub>3</sub> Pd <sub>2</sub> , Al <sub>3</sub> Pt <sub>2</sub> , Al <sub>2</sub> Si <sub>2</sub> Y, Cs <sub>2</sub> F <sub>6</sub> Nb, Al <sub>13</sub> Ba <sub>7</sub> , Cs <sub>2</sub> F <sub>6</sub> NaTi, N <sub>2</sub> Zr, HfTe <sub>2</sub> , LiS <sub>2</sub> Ti, NbSe <sub>2</sub> , LiS <sub>2</sub> Sn, NbTe <sub>2</sub> , OTi <sub>2</sub> , LiSe <sub>2</sub> Zr, LiTe <sub>2</sub> Ti, Ga <sub>3</sub> Pt <sub>2</sub> , In <sub>3</sub> Pd <sub>2</sub> , In <sub>3</sub> Pt <sub>2</sub> , Se <sub>2</sub> Ti, S <sub>2</sub> Ta, Se <sub>2</sub> Ta, O <sub>2</sub> PTi <sub>3</sub> , Sb <sub>2</sub> SrZn <sub>2</sub> , In <sub>4</sub> Li <sub>5</sub> , F <sub>6</sub> NbRb <sub>2</sub> , Hg <sub>7</sub> K <sub>2</sub> , Hg <sub>7</sub> Rb <sub>2</sub> , Li <sub>13</sub> Sn <sub>5</sub> , MoN, Pd <sub>13</sub> Tl <sub>9</sub> , Mo <sub>6</sub> O <sub>17</sub> Tl, Ge <sub>7</sub> Nb <sub>10</sub> , Au <sub>2</sub> U, Cd <sub>2</sub> Lu, Al <sub>2</sub> Ge <sub>2</sub> La, Al <sub>2</sub> Ge <sub>2</sub> Lu, Cd <sub>2</sub> La, AsN <sub>2</sub> U <sub>2</sub> , Br <sub>2</sub> La <sub>2</sub> P, N <sub>2</sub> PU <sub>2</sub> , Hg <sub>2</sub> La, N <sub>2</sub> SeU <sub>2</sub> , N <sub>3</sub> Th <sub>2</sub> , N <sub>3</sub> U <sub>2</sub> , I <sub>2</sub> La <sub>2</sub> P, ReTi <sub>2</sub> , F <sub>6</sub> K <sub>2</sub> Re, CdGaInS <sub>4</sub> ,
<b>165</b>	Ba, AsLi <sub>3</sub> , AuMg <sub>3</sub> , La <sub>5</sub> O <sub>15</sub> Ti <sub>4</sub> , F <sub>30</sub> GaNa <sub>3</sub> U <sub>6</sub> ,
<b>166</b>	HgIn, Se <sub>2</sub> Ta, PTe <sub>2</sub> Ti <sub>2</sub> , Au <sub>7</sub> Cs <sub>4</sub> Sn <sub>2</sub> , Al <sub>2</sub> Li <sub>3</sub> , Ba <sub>2</sub> N, LiPb, AgInSe <sub>2</sub> , B <sub>3</sub> Mo, HgNa <sub>3</sub> , Li, Ga <sub>2</sub> Li <sub>3</sub> , LiMoO <sub>2</sub> , In <sub>2</sub> Li <sub>3</sub> , F <sub>3</sub> Ti, LiS <sub>2</sub> Sn, Ge <sub>2</sub> Li <sub>4</sub> Zr, In <sub>2</sub> Se <sub>3</sub> , Se, Ca <sub>2</sub> N, Po, Te, GeTe, S, NbS <sub>2</sub> , GeP <sub>3</sub> , MoNaO <sub>2</sub> , NSr <sub>2</sub> , LiS <sub>2</sub> Ti, As <sub>2</sub> NaSn <sub>2</sub> , In <sub>3</sub> Te <sub>4</sub> , KS <sub>2</sub> Ti, Na, Cd <sub>4</sub> KP <sub>3</sub> , NaS <sub>2</sub> Ti, B <sub>5</sub> Mo <sub>2</sub> , KS <sub>2</sub> Sn, KS <sub>2</sub> Zr, NaS <sub>2</sub> Sn, RbS <sub>2</sub> Sn, Li <sub>5</sub> Tl <sub>2</sub> , Li <sub>5</sub> Sn <sub>2</sub> , Y <sub>2</sub> Zn <sub>17</sub> , B <sub>5</sub> W <sub>2</sub> , Na <sub>5</sub> Pb <sub>2</sub> , PTe <sub>2</sub> Zr <sub>2</sub> , Be <sub>3</sub> Ti, Be <sub>3</sub> Nb, As <sub>3</sub> Sn <sub>4</sub> , Na <sub>5</sub> Sn <sub>2</sub> , As <sub>3</sub> NaZn <sub>4</sub> , Be <sub>3</sub> Ta, P <sub>3</sub> Sn <sub>4</sub> , Pb <sub>2</sub> Pd <sub>3</sub> Se <sub>2</sub> , Pd <sub>3</sub> Se <sub>2</sub> Tl <sub>2</sub> , Bi <sub>3</sub> Se <sub>4</sub> , P <sub>3</sub> Sn, Pb <sub>2</sub> Pd <sub>3</sub> S <sub>2</sub> , Be <sub>17</sub> Nb <sub>2</sub> , Ga <sub>7</sub> Rb, Be <sub>17</sub> Zr <sub>2</sub> , Be <sub>17</sub> Ti <sub>2</sub> , Bi <sub>4</sub> Te <sub>3</sub> , Al <sub>3</sub> Y, CsGa <sub>7</sub> , Be <sub>17</sub> Ta <sub>2</sub> , Be <sub>17</sub> Hf <sub>2</sub> , Sn <sub>3</sub> Sr, SbSn, Ag <sub>2</sub> Al <sub>7</sub> Ca <sub>3</sub> , B <sub>13</sub> N <sub>2</sub> , C <sub>2</sub> B <sub>12</sub> Be, C <sub>2</sub> B <sub>13</sub> , C <sub>3</sub> Al <sub>8</sub> N <sub>4</sub> , Al <sub>9</sub> Sr <sub>5</sub> , BaPb <sub>3</sub> , Au <sub>7</sub> Rb <sub>4</sub> Sn <sub>2</sub> , Au <sub>7</sub> Ge <sub>2</sub> K <sub>4</sub> , Li <sub>5</sub> Na <sub>2</sub> Sn <sub>4</sub> , Cs <sub>4</sub> OTl <sub>2</sub> , CCl <sub>2</sub> La <sub>2</sub> , Lu, NU, LiO <sub>3</sub> U, Ge <sub>3</sub> La, Th <sub>2</sub> Zn <sub>17</sub> , PU, CB <sub>2</sub> U, La <sub>2</sub> Zn <sub>17</sub> , Lu <sub>2</sub> Zn <sub>17</sub> , U <sub>2</sub> Zn <sub>17</sub> , O <sub>6</sub> PbRe <sub>2</sub> , Ag <sub>4</sub> Sb <sub>2</sub> Sr,
<b>167</b>	Au <sub>6</sub> Sr <sub>2</sub> Zn <sub>3</sub> , HgO <sub>3</sub> Sn, NPd <sub>3</sub> , F <sub>3</sub> Ti, F <sub>3</sub> Pd, F <sub>3</sub> Mo, Al <sub>5</sub> Mo, OZr <sub>3</sub> , O <sub>3</sub> Ti <sub>2</sub> , BO <sub>3</sub> Ti, Au <sub>6</sub> Ga <sub>3</sub> Sr <sub>2</sub> , Cd <sub>6</sub> Sb <sub>5</sub> , Ga <sub>5</sub> NSr <sub>6</sub> , Hg <sub>3</sub> Na <sub>8</sub> , Al <sub>3</sub> Au <sub>8</sub> , Ba <sub>6</sub> Ga <sub>5</sub> N, Mo <sub>9</sub> S <sub>11</sub> Tl <sub>2</sub> , Ba <sub>6</sub> In <sub>5</sub> N, K <sub>8</sub> Tl <sub>11</sub> , K <sub>2</sub> Mo <sub>9</sub> S <sub>11</sub> , Mo <sub>9</sub> Rb <sub>2</sub> S <sub>11</sub> , In <sub>11</sub> K <sub>8</sub> , Rb <sub>8</sub> Tl <sub>11</sub> , In <sub>11</sub> Rb <sub>8</sub> , Mo <sub>15</sub> Na <sub>2</sub> Se <sub>19</sub> , Cs <sub>8</sub> Ga <sub>11</sub> , Ba <sub>14</sub> CaN <sub>6</sub> Na <sub>7</sub> , Ba <sub>2</sub> Mo <sub>15</sub> Se <sub>19</sub> , Mg <sub>21</sub> Zn <sub>25</sub> , Mo <sub>15</sub> Pb <sub>2</sub> Se <sub>19</sub> , Mo <sub>15</sub> Rb <sub>2</sub> S <sub>19</sub> , Mo <sub>15</sub> Se <sub>19</sub> Sn <sub>2</sub> , Li <sub>2</sub> Mo <sub>15</sub> Se <sub>19</sub> , K <sub>2</sub> Mo <sub>15</sub> Se <sub>19</sub> , In <sub>2</sub> Mo <sub>15</sub> Se <sub>19</sub> , K <sub>2</sub> Mo <sub>15</sub> S <sub>19</sub> , Cs <sub>2</sub> Mo <sub>15</sub> S <sub>19</sub> , Mo <sub>21</sub> Rb <sub>4</sub> S <sub>25</sub> , Ca <sub>6</sub> Hf <sub>19</sub> O <sub>44</sub> ,
<b>173</b>	Al <sub>5</sub> Mo, Al <sub>5</sub> W, AlCaSi, CaO <sub>11</sub> Ta <sub>4</sub> , Cl <sub>3</sub> KTi, I <sub>3</sub> KTi, BeGaLa <sub>3</sub> S <sub>7</sub> , AlLa <sub>3</sub> S <sub>7</sub> Ti, BeInLa <sub>3</sub> S <sub>7</sub> , BeLa <sub>3</sub> LuS <sub>7</sub> ,
<b>174</b>	Al <sub>3</sub> Zr <sub>4</sub> , NTa, As <sub>7</sub> Nb <sub>9</sub> Pd, Te <sub>12</sub> U <sub>7</sub> , O <sub>2</sub> Se <sub>12</sub> U <sub>7</sub> , B <sub>3</sub> BrLa <sub>2</sub> ,
<b>176</b>	Mo <sub>15</sub> S <sub>19</sub> Sn <sub>2</sub> , NbSe <sub>2</sub> , BaMo <sub>3</sub> Te <sub>3</sub> , CsMo <sub>3</sub> Te <sub>3</sub> , CsMo <sub>3</sub> S <sub>3</sub> , KM <sub>0</sub> <sub>3</sub> Se <sub>3</sub> , Mo <sub>3</sub> RbS <sub>3</sub> , Mo <sub>3</sub> NaTe <sub>3</sub> , Mo <sub>3</sub> RbSe <sub>3</sub> , LiMo <sub>3</sub> Se <sub>3</sub> , Nb <sub>3</sub> S <sub>4</sub> , BaMo <sub>3</sub> Se <sub>3</sub> , AsNb <sub>3</sub> Te <sub>3</sub> , InMo <sub>3</sub> Te <sub>3</sub> , KM <sub>0</sub> <sub>3</sub> Te <sub>3</sub> , Mo <sub>3</sub> RbTe <sub>3</sub> , Nb <sub>3</sub> Te <sub>4</sub> , Nb <sub>3</sub> Se <sub>4</sub> , AgMo <sub>3</sub> Se <sub>3</sub> , InMo <sub>3</sub> Se <sub>3</sub> , CsMo <sub>3</sub> Se <sub>3</sub> , Mo <sub>6</sub> Se <sub>6</sub> Tl <sub>2</sub> , Mo <sub>3</sub> NaSe <sub>3</sub> , KM <sub>0</sub> <sub>3</sub> S <sub>3</sub> , Se <sub>4</sub> Ti <sub>3</sub> , Mo <sub>3</sub> Se <sub>3</sub> Tl, Au <sub>10</sub> In <sub>3</sub> , AgNb <sub>3</sub> Te <sub>4</sub> , Au <sub>10</sub> Ga <sub>16</sub> Na <sub>5</sub> , AgCd <sub>3</sub> F <sub>20</sub> Hf <sub>3</sub> , AgCd <sub>3</sub> F <sub>20</sub> Zr <sub>3</sub> , K <sub>3</sub> Mg <sub>18</sub> Sn <sub>11</sub> , Mo <sub>15</sub> Se <sub>19</sub> , K <sub>3</sub> Mg <sub>18</sub> Pb <sub>11</sub> , Mo <sub>15</sub> Rb <sub>3</sub> Se <sub>17</sub> , Mo <sub>15</sub> Pb <sub>2</sub> Se <sub>19</sub> , Li <sub>5</sub> Mo <sub>15</sub> S <sub>19</sub> , Cs <sub>3</sub> Mo <sub>15</sub> Se <sub>17</sub> , Cs <sub>3</sub> Mo <sub>15</sub> Te <sub>17</sub> , CCl <sub>18</sub> LiW <sub>6</sub> , CCl <sub>18</sub> NaW <sub>6</sub> , Mo <sub>27</sub> Rb <sub>5</sub> Se <sub>31</sub> , Cl <sub>3</sub> U, Br <sub>3</sub> U,
<b>180</b>	Si <sub>2</sub> Ta, MoSn <sub>2</sub> , BLuPt <sub>2</sub> ,
<b>181</b>	Si <sub>2</sub> Ta,

Part 8 of all the predicted **Case 3-TSMs**:

<b>182</b>	Nb <sub>3</sub> S <sub>6</sub> Ti, IO <sub>6</sub> PbRb, CsI <sub>11</sub> Nb <sub>6</sub> ,
<b>185</b>	Mg <sub>3</sub> Pd, AuCd <sub>3</sub> , Mg <sub>3</sub> Pt, F <sub>3</sub> U,
<b>186</b>	InSb, NZr, Ge, NPD, GaSb, AuScSn, AgSnY, CaSnZn, AuSnY, AuGeY, CaHgSn, AgBiCa, CSc, HgSnSr, HgPbSr, C <sub>4</sub> Al <sub>3</sub> Zr <sub>2</sub> , Au <sub>3</sub> LiSn <sub>4</sub> , C <sub>5</sub> Al <sub>3</sub> Zr <sub>3</sub> , Mo <sub>3</sub> O <sub>8</sub> ScZn, Au <sub>3</sub> Sr <sub>7</sub> , Ag <sub>3</sub> Sr <sub>7</sub> , LiSbSn, LiSnY, InLi <sub>2</sub> Mo <sub>3</sub> O <sub>8</sub> , Ca <sub>5</sub> Pb <sub>3</sub> , AgLaPb, AuSnU, AuGeLa, AuLuSn, AgLuSn, AuGeLu, AuLaSn, C <sub>3</sub> Al <sub>3</sub> U, C <sub>4</sub> Al <sub>3</sub> U <sub>2</sub> , La <sub>7</sub> Pd <sub>3</sub> , Pt <sub>3</sub> Th <sub>7</sub> , La <sub>7</sub> Pt <sub>3</sub> , LiLuSn, Cd <sub>4</sub> La <sub>23</sub> Pt <sub>7</sub> , B <sub>3</sub> Re <sub>7</sub> , B <sub>3</sub> Re <sub>7</sub> ,
<b>187</b>	CAu, CdN, PbSe <sub>2</sub> Ta, NTa, Se <sub>2</sub> Ta, AgN, AlSn, AlGeSr, AlCaSi, AlBaSi, AsBaPd, CW, AlSiSr, AlBaGe, CMo, BaLiSi, CTa, CPt, LiPd, NNb, MoP, NPD, NZr, NW, NbS, STi, TeZr, STa, InS <sub>2</sub> Ta, N <sub>2</sub> Pt, PtSbSr, InSe <sub>2</sub> Ta, N <sub>2</sub> Ta, Al <sub>5</sub> Ba <sub>5</sub> Pb, Ba <sub>5</sub> Ga <sub>5</sub> Pb, CsO <sub>2</sub> Y, GeLiZn, CaLiPb, Al <sub>5</sub> Ba <sub>5</sub> Sn, Au <sub>4</sub> In <sub>6</sub> K, Au <sub>4</sub> In <sub>6</sub> Rb, Ba <sub>5</sub> Ga <sub>5</sub> Sn, CLiNaO <sub>3</sub> , CLa, AuSiTh, AuSiU, Mo <sub>13</sub> P <sub>9</sub> U, NRe, N <sub>2</sub> Re, NRe <sub>3</sub> , ReSe <sub>2</sub> , U <sub>2</sub> Zn <sub>17</sub> ,
<b>188</b>	I <sub>3</sub> LiSc, LaNO <sub>2</sub> Si,
<b>189</b>	GePt <sub>2</sub> , Ag <sub>2</sub> Ga, InMg <sub>2</sub> , InPtY, AsPd <sub>2</sub> , Mg <sub>2</sub> Tl, NTa, Li <sub>2</sub> Sb, PdYZn, BGe <sub>2</sub> Ti <sub>6</sub> , Hf <sub>5</sub> Sc, PdScSn, AlPdY, GePdSc, GePd <sub>2</sub> , GaPtZr, Al <sub>2</sub> Hf <sub>6</sub> Pt, AuInY, AlPtZr, HfMoP, AlHfPt, Pt <sub>2</sub> Si, MgPdY, BSi <sub>2</sub> Ti <sub>6</sub> , InPdY, InPtSc, SiY, MoPzr, MgYZn, PdTiY, Pd <sub>2</sub> Si, PtSnY, PbPdY, PtSb <sub>2</sub> Zr <sub>6</sub> , PtScSn, Au <sub>7</sub> Ga <sub>2</sub> , In <sub>4</sub> Pt <sub>3</sub> Sr <sub>2</sub> , Cd <sub>9</sub> K <sub>14</sub> Tl <sub>21</sub> , Cs <sub>15</sub> Tl <sub>27</sub> , PTi <sub>2</sub> , HgLaPd, InPtU, InLaPd, InPtTh, InPdU, InLuPd, InPdTh, LuPdZn, LaPtSn, GaPdU, InLuPt, AlPdTh, LuPdSn, AuInLu, S <sub>2</sub> U, CdLaPd, AlAuLu, AlLuPd, AgLuPb, AuInLa, LaPdSn, GaPtTh, GaPtU, LaPdTl, AlPtU, LaPbPd, LaMgPd, LuPtSn, Lu <sub>8</sub> Te, Al <sub>13</sub> La <sub>16</sub> , ReSiTi, ReSiTa, NbReSi, C <sub>15</sub> Re <sub>5</sub> Y <sub>12</sub> ,
<b>190</b>	GaMg <sub>2</sub> , PdScSn, GaPtZr, GaHfPd, Li <sub>2</sub> Sb, AlPtZr, AlHfPt, PtScSn, B <sub>4</sub> Ga <sub>3</sub> Pt <sub>9</sub> , Ge <sub>2</sub> O <sub>13</sub> Rb <sub>3</sub> U <sub>3</sub> , K <sub>3</sub> O <sub>13</sub> Si <sub>2</sub> U <sub>3</sub> ,
<b>191</b>	AlB <sub>2</sub> , Ag <sub>5</sub> Sr, Au <sub>2</sub> Ba, AuB <sub>2</sub> , Ag <sub>5</sub> Ba, B <sub>2</sub> Nb, B <sub>2</sub> Sc, Al <sub>3</sub> Hf <sub>4</sub> , Au <sub>2</sub> Nb, Au <sub>5</sub> K, B <sub>2</sub> Ta, B <sub>2</sub> Mo, Al <sub>3</sub> Zr <sub>4</sub> , B <sub>2</sub> Y, Au <sub>5</sub> Ba, Au <sub>5</sub> Sr, CaGa <sub>2</sub> , Be <sub>5</sub> Zr, Bi <sub>2</sub> Tl, Be <sub>5</sub> Hf, Be <sub>2</sub> Zr, Be <sub>2</sub> Hf, Be <sub>5</sub> Sc, BaPd <sub>5</sub> , Hg, Hf, CaHg <sub>2</sub> , NNa <sub>3</sub> , Ga <sub>2</sub> Y, Li <sub>2</sub> NNa, Hg <sub>2</sub> Na, BaGa <sub>2</sub> , Hg <sub>2</sub> Y, Si <sub>2</sub> Y, LiNNa <sub>2</sub> , CaPt <sub>5</sub> , S <sub>2</sub> Ti, Rf, N <sub>3</sub> TaTi <sub>2</sub> , Hg <sub>2</sub> Sr, Hf <sub>2</sub> N <sub>3</sub> Ta, N <sub>3</sub> OTa <sub>2</sub> , N <sub>4</sub> Ta <sub>2</sub> , ScSi <sub>2</sub> , N <sub>3</sub> Ta <sub>2</sub> Ti, NTa, PtTl, Au <sub>5</sub> Rb, C <sub>6</sub> Li, Pt <sub>5</sub> Sr, SrZn <sub>5</sub> , BN <sub>3</sub> Ta <sub>2</sub> , YZn <sub>5</sub> , CN <sub>3</sub> Ta <sub>2</sub> , N <sub>3</sub> TaZr <sub>2</sub> , C <sub>12</sub> Li, BaPt <sub>5</sub> , N <sub>3</sub> Ta <sub>2</sub> Zr, NOTa, Ag <sub>7</sub> Te <sub>4</sub> , Si <sub>2</sub> U, Ga <sub>2</sub> La, Si <sub>2</sub> Th, TiU <sub>2</sub> , ThZn <sub>2</sub> , Cd <sub>2</sub> Th, C <sub>3</sub> Si <sub>16</sub> U <sub>20</sub> ,
<b>193</b>	BGe <sub>3</sub> Ta <sub>5</sub> , Au <sub>6</sub> Hg <sub>5</sub> , BGe <sub>3</sub> Nb <sub>5</sub> , Br <sub>3</sub> Zr, Cl <sub>3</sub> Ti, AgSb <sub>3</sub> Zr <sub>5</sub> , AsPb <sub>3</sub> Zr <sub>5</sub> , Ga <sub>3</sub> Nb <sub>5</sub> , AsSb <sub>3</sub> Zr <sub>5</sub> , AlSn <sub>3</sub> Zr <sub>5</sub> , I <sub>3</sub> Ti, Ga <sub>4</sub> Ti <sub>5</sub> , I <sub>3</sub> Nb, Cl <sub>3</sub> Zr, As <sub>3</sub> Sr <sub>5</sub> , CSb <sub>3</sub> Zr <sub>5</sub> , Ga <sub>3</sub> Ti <sub>5</sub> , Ga <sub>4</sub> Zr <sub>5</sub> , GaSn <sub>3</sub> Zr <sub>5</sub> , P <sub>3</sub> Ti <sub>5</sub> , Nb <sub>5</sub> Si <sub>3</sub> , CSn <sub>3</sub> Zr <sub>5</sub> , InPb <sub>3</sub> Zr <sub>5</sub> , In <sub>3</sub> Y <sub>5</sub> , Al <sub>3</sub> Zr <sub>5</sub> , Al <sub>3</sub> Hf <sub>5</sub> , SSb <sub>3</sub> Zr <sub>5</sub> , Pb <sub>3</sub> SbZr <sub>5</sub> , NSn <sub>3</sub> Zr <sub>5</sub> , Al <sub>3</sub> Y <sub>5</sub> , Ba <sub>3</sub> N, AgIn <sub>3</sub> Zr <sub>5</sub> , AsSn <sub>3</sub> Zr <sub>5</sub> ,

Part 9 of all the predicted **Case 3-TSMs**:

193	Pb <sub>3</sub> Sc <sub>5</sub> , HfI <sub>3</sub> , Pt <sub>3</sub> Zr <sub>5</sub> , Pb <sub>3</sub> Y <sub>5</sub> , Ge <sub>3</sub> Mo <sub>5</sub> , Sb <sub>4</sub> Zr <sub>5</sub> , Ba <sub>5</sub> Bi <sub>3</sub> , BNb <sub>5</sub> Si <sub>3</sub> , Sb <sub>3</sub> Zr <sub>5</sub> , Pb <sub>3</sub> SnZr <sub>5</sub> , I <sub>3</sub> Zr, Al <sub>3</sub> Ta <sub>5</sub> , Sc <sub>5</sub> Si <sub>3</sub> , Ga <sub>4</sub> Nb <sub>5</sub> , Sn <sub>3</sub> ZnZr <sub>5</sub> , Ge <sub>3</sub> Nb <sub>5</sub> , SiSn <sub>3</sub> Zr <sub>5</sub> , Ga <sub>3</sub> Ti <sub>2</sub> Zr <sub>3</sub> , Sn <sub>3</sub> Y <sub>5</sub> , Ga <sub>3</sub> Zr <sub>5</sub> , Mo <sub>5</sub> Si <sub>3</sub> , Sb <sub>3</sub> Y <sub>5</sub> , Si <sub>3</sub> Ta <sub>5</sub> , BSn <sub>3</sub> Zr <sub>5</sub> , CdPb <sub>3</sub> Zr <sub>5</sub> , Ga <sub>3</sub> Hf <sub>3</sub> Nb <sub>2</sub> , Hg <sub>3</sub> Mg <sub>5</sub> , Pb <sub>3</sub> SiZr <sub>5</sub> , Ga <sub>3</sub> Sc <sub>5</sub> , Sn <sub>4</sub> Zr <sub>5</sub> , Sb <sub>3</sub> Si <sub>5</sub> , Ca <sub>5</sub> Sb <sub>3</sub> , AgPb <sub>3</sub> Zr <sub>5</sub> , Al <sub>4</sub> Zr <sub>5</sub> , Nb <sub>5</sub> PSi <sub>3</sub> , N <sub>6</sub> Ta <sub>5</sub> , Hf <sub>5</sub> Sb <sub>3</sub> Zn, Ge <sub>3</sub> Sc <sub>5</sub> , Sc <sub>5</sub> Sn <sub>3</sub> , Ga <sub>3</sub> Y <sub>5</sub> , Ge <sub>3</sub> Ta <sub>5</sub> , Pb <sub>3</sub> SeZr <sub>5</sub> , Sb <sub>3</sub> SiZr <sub>5</sub> , As <sub>3</sub> Ca <sub>5</sub> , PPb <sub>3</sub> Zr <sub>5</sub> , Ge <sub>3</sub> Y <sub>5</sub> , N <sub>6</sub> Nb <sub>5</sub> , Si <sub>3</sub> Y <sub>5</sub> , Ga <sub>3</sub> Ta <sub>5</sub> , Tl <sub>3</sub> Y <sub>5</sub> , SSn <sub>3</sub> Zr <sub>5</sub> , Bi <sub>3</sub> Sr <sub>5</sub> , PSn <sub>3</sub> Zr <sub>5</sub> , GePb <sub>3</sub> Zr <sub>5</sub> , Hf <sub>5</sub> Si <sub>3</sub> , Al <sub>3</sub> Hf <sub>5</sub> N, Sb <sub>3</sub> SeZr <sub>5</sub> , SeSn <sub>3</sub> Zr <sub>5</sub> , Hf <sub>5</sub> Sn <sub>3</sub> , Pt <sub>3</sub> Y <sub>5</sub> , Nb <sub>5</sub> OPT <sub>3</sub> , Hf <sub>5</sub> Sn <sub>4</sub> , Ba <sub>5</sub> Sb <sub>3</sub> , K <sub>3</sub> Nb <sub>8</sub> O <sub>21</sub> , Au <sub>41</sub> Mg <sub>13</sub> , Al <sub>43</sub> Mo <sub>4</sub> Y <sub>6</sub> , Ga <sub>3</sub> Lu <sub>5</sub> , Bi <sub>5</sub> La <sub>3</sub> Sc, Ge <sub>3</sub> La <sub>5</sub> , La <sub>5</sub> Si <sub>3</sub> , In <sub>3</sub> Lu <sub>5</sub> , La <sub>5</sub> Sb <sub>3</sub> , BrLa <sub>5</sub> Sn <sub>3</sub> , La <sub>5</sub> Pb <sub>3</sub> Zn, La <sub>5</sub> PPb <sub>3</sub> , La <sub>5</sub> Pb <sub>3</sub> Se, CGe <sub>3</sub> Lu <sub>5</sub> , Lu <sub>5</sub> Sn <sub>3</sub> , Ge <sub>3</sub> U <sub>5</sub> , Lu <sub>5</sub> Tl <sub>3</sub> , Pb <sub>3</sub> Th <sub>5</sub> , Lu <sub>5</sub> Si <sub>3</sub> , Bi <sub>5</sub> La <sub>3</sub> Mg, La <sub>5</sub> Pb <sub>3</sub> S, Sb <sub>5</sub> TiU <sub>3</sub> , Sb <sub>5</sub> ScU <sub>3</sub> , Ge <sub>3</sub> Lu <sub>5</sub> , Lu <sub>5</sub> Pb <sub>3</sub> , HfSb <sub>5</sub> U <sub>3</sub> , Sb <sub>5</sub> U <sub>3</sub> Zr, Lu <sub>5</sub> Pt <sub>3</sub> , CLa <sub>5</sub> Pb <sub>3</sub> , La <sub>3</sub> Sb <sub>5</sub> Zr, HfLa <sub>3</sub> Sn <sub>5</sub> , AgLa <sub>5</sub> Pb <sub>3</sub> , La <sub>5</sub> Pb <sub>3</sub> Sb, BrLa <sub>5</sub> Sb <sub>3</sub> , CLa <sub>5</sub> Sn <sub>3</sub> , La <sub>5</sub> Pb <sub>3</sub> , Bi <sub>3</sub> BrLa <sub>5</sub> , AsLa <sub>5</sub> Pb <sub>3</sub> , Bi <sub>3</sub> La <sub>5</sub> , CLa <sub>5</sub> Sn <sub>3</sub> , La <sub>3</sub> Sb <sub>5</sub> Ti, Sn <sub>4</sub> Th <sub>5</sub> , Pb <sub>4</sub> Th <sub>5</sub> , ILa <sub>5</sub> Pb <sub>3</sub> , BrIn <sub>3</sub> La <sub>5</sub> , Al <sub>3</sub> Ba <sub>10</sub> Ge <sub>7</sub> ,
194	B <sub>5</sub> W <sub>2</sub> , BaNbS <sub>3</sub> , C <sub>5</sub> Al <sub>3</sub> Zr <sub>3</sub> , BW <sub>4</sub> Zr <sub>9</sub> , Hf <sub>9</sub> Mo <sub>4</sub> P, Cs <sub>6</sub> K <sub>7</sub> , Pb, Si, NbS, Ti, SeZr <sub>2</sub> , Sb, Sc, Tl, Y, STi, Zr, PdSb, PdTe, Sr, PoTi, TeTi, SeTi, TeZr, PtSb, PtTe, PoSc, SbTi, ScTe, NbS <sub>2</sub> , PbSrZn, PZr, NaTl, SrTl <sub>2</sub> , S <sub>2</sub> Ta, NbSe <sub>2</sub> , Se <sub>2</sub> Ta, NbPbS <sub>2</sub> , PTi, O <sub>2</sub> , PbS <sub>2</sub> Ta, TiZn <sub>2</sub> , Pt <sub>2</sub> SnY, NbS <sub>2</sub> Sn, S <sub>2</sub> SnTa, PSbZr <sub>2</sub> , PSbTl <sub>2</sub> , SrZn <sub>2</sub> , SnYZn, Pd <sub>3</sub> Ti, Pd <sub>3</sub> Zr, Pt <sub>2</sub> Sn <sub>3</sub> , Pt <sub>2</sub> Si <sub>3</sub> , Pt <sub>2</sub> Sn <sub>2</sub> Zn <sub>3</sub> , Sn <sub>5</sub> Ti <sub>6</sub> , NbZn <sub>2</sub> , Ag, AgBiCa, AgAsBa, AlZr <sub>2</sub> , AlSc <sub>2</sub> , AlYZn, AlPt <sub>2</sub> Zr, AlHfPt <sub>2</sub> , AlPtTi, Al <sub>3</sub> Y, AsAuBa, AgBaBi, AgAsSr, AsPdSr, AsHf, AsZr, AgBiSr, Nb <sub>4</sub> S <sub>8</sub> Ti, Ag <sub>2</sub> K, AuLiSn, AuCaSb, AuBaSb, AuBiSr, AuNaTe, AuSe, AuSn, AuRbTe, AuBaP, BLi, AuSbSr, AsTi, Al <sub>2</sub> NaO <sub>6</sub> Sb, AuKTe, Al <sub>4</sub> Mg <sub>2</sub> Zn <sub>3</sub> , BaCdGe, BaGeZn, B <sub>4</sub> Mo, BaHgSn, BaPt, AuCaP, BPt <sub>2</sub> , AsPtSr, Au <sub>2</sub> K, BiPd, BiPt, AuSnY, BaPbZn, BiIn <sub>2</sub> , BaTl <sub>2</sub> , Au <sub>3</sub> LiNa <sub>2</sub> , BiNa <sub>3</sub> , AuMg <sub>3</sub> , BaSiZn, BaMg <sub>2</sub> , CAITi <sub>2</sub> , Ba <sub>3</sub> LiN, CAISc <sub>2</sub> , CNb, CGaTi <sub>2</sub> , BaSe <sub>3</sub> Ta, CSc, CAsNb <sub>2</sub> , BaSn <sub>3</sub> , CInZr <sub>2</sub> , BiRb <sub>3</sub> , Br <sub>3</sub> RbTi, CMo, BiK <sub>3</sub> , CGaNb <sub>2</sub> , AlN <sub>3</sub> Ta <sub>4</sub> , CPTa <sub>2</sub> , CSTi <sub>2</sub> , CGaSc <sub>2</sub> , Br <sub>3</sub> CsTi, CAInNb <sub>2</sub> , CSZr <sub>2</sub> , CInTa <sub>2</sub> , CInTi <sub>2</sub> , YZn <sub>5</sub> , CSc <sub>2</sub> Tl, Ca, CGaMo <sub>2</sub> , CTiZr <sub>2</sub> , C <sub>2</sub> S <sub>2</sub> Ti <sub>4</sub> , C <sub>2</sub> S <sub>2</sub> Zr <sub>4</sub> , CSiTi <sub>2</sub> , CaHgSn, Al <sub>5</sub> Ba <sub>4</sub> , CaIn <sub>2</sub> , CaHgPb, Ba <sub>3</sub> NNa, CdN, CaPbZn, B <sub>4</sub> W, CaGa <sub>2</sub> , CInSc <sub>2</sub> , CdS <sub>2</sub> Ta, CAITa <sub>2</sub> , BaS <sub>3</sub> Ta, CHf <sub>2</sub> S, CAIW <sub>2</sub> , CaSnZn, Cd <sub>3</sub> Mg, CAIZr <sub>2</sub> , C <sub>2</sub> GeTi <sub>3</sub> , CNb <sub>2</sub> P, CaLi <sub>2</sub> , CGaTa <sub>2</sub> , CInNb <sub>2</sub> , CTi <sub>2</sub> Tl, Cd <sub>3</sub> Sc, CHf <sub>2</sub> Tl, GaPtTi, CHf <sub>2</sub> In, B <sub>5</sub> Mo <sub>2</sub> , Ge, CaZn <sub>2</sub> , Hf, Cl <sub>3</sub> CsTi, CaMg <sub>2</sub> , GaTi <sub>2</sub> , GaYZn, HfPo, CaCd <sub>2</sub> , Cl <sub>3</sub> CsSc, CaPt <sub>2</sub> , GeMg <sub>2</sub> , Be <sub>17</sub> Ti <sub>2</sub> , Ga <sub>2</sub> Mg, Be <sub>17</sub> Hf <sub>2</sub> , Y <sub>2</sub> Zn <sub>17</sub> , Cl <sub>3</sub> RbTi, GaTi <sub>3</sub> , CaHg <sub>3</sub> , C <sub>3</sub> AlNb <sub>4</sub> , HgMg <sub>3</sub> , K, InMoS <sub>2</sub> , Hg <sub>3</sub> Y, AuNa <sub>2</sub> Sn <sub>3</sub> , Li, Hf <sub>2</sub> S, Hg <sub>3</sub> Li, C <sub>4</sub> Al <sub>3</sub> Zr <sub>2</sub> , InY <sub>2</sub> , In <sub>2</sub> Sr, InMg <sub>3</sub> , GaNTi <sub>2</sub> , InSc <sub>2</sub> , In <sub>3</sub> Sr, Hg <sub>3</sub> Sc, Li <sub>2</sub> SiZn, GeYZn, C <sub>2</sub> AlTi <sub>3</sub> , Mg <sub>2</sub> Sn, N <sub>2</sub> , NTa, NZr, MgZn <sub>2</sub> , NNb, InTi <sub>3</sub> , Mg <sub>2</sub> Si, Na, NPt, NPd, Hg <sub>3</sub> Sr, InS <sub>2</sub> W, MoN, InSc <sub>3</sub> , MgNa <sub>2</sub> Pb, Mg <sub>3</sub> Pt, Hf <sub>2</sub> PSb, Mg <sub>3</sub> Pd, KSn <sub>2</sub> , MgNa <sub>2</sub> Sn,

Part 10 of all the predicted **Case 3-TSMs**:

	LiTl, KPb <sub>2</sub> , C <sub>3</sub> AlTa <sub>4</sub> , Mg <sub>2</sub> PtSi, N <sub>2</sub> Ta, C <sub>4</sub> Al <sub>3</sub> Hf <sub>2</sub> , N <sub>3</sub> W <sub>2</sub> , Pd <sub>3</sub> Ta, B <sub>4</sub> Ta, BaNa <sub>2</sub> , BMo <sub>4</sub> Zr <sub>9</sub> , KNa <sub>2</sub> , CsI <sub>3</sub> Ti, BaLi <sub>4</sub> , CaNa <sub>4</sub> Sn <sub>6</sub> , Ga <sub>5</sub> Ta <sub>6</sub> , Mg <sub>2</sub> Y, Mg <sub>2</sub> Sr, HfZn <sub>2</sub> , N <sub>2</sub> Pt, AsHf <sub>9</sub> Mo <sub>4</sub> , Li <sub>3</sub> Sn <sub>4</sub> Zn <sub>2</sub> , C <sub>6</sub> Al <sub>3</sub> Zr <sub>4</sub> , C <sub>5</sub> Al <sub>3</sub> Hf <sub>3</sub> , AsHf <sub>9</sub> W <sub>4</sub> , HfMo <sub>2</sub> , GeHf <sub>9</sub> Mo <sub>4</sub> , Mg <sub>5</sub> Pd <sub>2</sub> , Hf <sub>9</sub> Mo <sub>4</sub> S, Hf <sub>9</sub> SW <sub>4</sub> , Hf <sub>10</sub> Mo <sub>3</sub> Si, Br <sub>9</sub> Nb <sub>2</sub> Rb <sub>3</sub> , Hf <sub>9</sub> SeW <sub>4</sub> , BHf <sub>9</sub> Mo <sub>4</sub> , Hf <sub>9</sub> Mo <sub>4</sub> Si, Hf <sub>9</sub> PW <sub>4</sub> , CsK <sub>7</sub> Rb <sub>5</sub> , Mg <sub>38</sub> Sr <sub>9</sub> , Cd <sub>3</sub> K <sub>16</sub> Na <sub>9</sub> Tl <sub>18</sub> , Cd <sub>58</sub> Y <sub>13</sub> , Hg <sub>58</sub> Sr <sub>13</sub> , Cd <sub>58</sub> Sr <sub>13</sub> , Al <sub>3</sub> Th, InLaZn, Lu, LaTlZn, Al <sub>3</sub> La, AsLaPd, Ga <sub>3</sub> Pd <sub>2</sub> U, CdLaTl, GeLaLi <sub>2</sub> , AlLa <sub>3</sub> , Hg <sub>2</sub> Th, Br <sub>2</sub> La, PdSbU, LaPdSb, InLaPd <sub>2</sub> , Hg <sub>3</sub> La, La, Cd <sub>3</sub> Th, InPt <sub>2</sub> U, Hg <sub>3</sub> Lu, PaPt <sub>3</sub> , AuLaSb, AuGeU, Pd <sub>3</sub> U, Al <sub>2</sub> U, U <sub>2</sub> Zn <sub>17</sub> , Th <sub>2</sub> Zn <sub>17</sub> , LuZn <sub>5</sub> , La <sub>2</sub> Mg <sub>17</sub> , Lu <sub>2</sub> Zn <sub>17</sub> , Cd <sub>17</sub> La <sub>2</sub> , B <sub>2</sub> Re, B <sub>3</sub> Re, NRe, CRe <sub>2</sub> , Re, Be <sub>2</sub> Re, CRe, C <sub>2</sub> Re, NRe <sub>2</sub> , N <sub>2</sub> Re, Re <sub>2</sub> W, B <sub>4</sub> Re, Re <sub>2</sub> Zr, GeHf <sub>9</sub> Re <sub>4</sub> , Hf <sub>9</sub> PRE <sub>4</sub> , N <sub>2</sub> O <sub>5</sub> , PRe <sub>4</sub> Zr <sub>9</sub> , BRe <sub>4</sub> Zr <sub>9</sub> , AsHf <sub>9</sub> Re <sub>4</sub> , Hf <sub>9</sub> Re <sub>4</sub> Si, BHf <sub>9</sub> Re <sub>4</sub> , Lu <sub>13</sub> Zn <sub>58</sub> , Cd <sub>58</sub> La <sub>13</sub> , AlTi <sub>3</sub> ,
194	B <sub>12</sub> ,
195	Li <sub>22</sub> Si <sub>5</sub> ,
196	Bi <sub>12</sub> O <sub>20</sub> Zn,
198	BaPdSi, AsPdS, BaPPt, Ba <sub>8</sub> Ga <sub>7</sub> , AlPd, AuBe, AlPt, BiPdSe, BiPdTe, AsPdSe, GaPd, BiPtTe, GaPt, AsBaPt, F <sub>2</sub> Pd, HfSb, AuGaNb <sub>3</sub> , HfSn, BiPtSe, AlAu <sub>4</sub> , BaGePt, BaPtSi, GePtSr, CaPtSi, PdSbSe, PdSSb, AuGaTa <sub>3</sub> , PdSbTe, PtSbSe, SbZr, PtSSb, PdSiSr, PtSiSr, Ga <sub>7</sub> Sr <sub>8</sub> , Al <sub>7</sub> Sr <sub>8</sub> , Al <sub>2</sub> Sr <sub>3</sub> , Ag <sub>9</sub> GaSe <sub>6</sub> , GaSr, ReSi, AlSr,
199	Bi <sub>2</sub> Pd <sub>3</sub> S <sub>2</sub> , Bi <sub>2</sub> Pt <sub>3</sub> Se <sub>2</sub> , N <sub>2</sub> O <sub>4</sub> ,
200	CdN <sub>3</sub> O <sub>6</sub> Tl, Po, HgN <sub>3</sub> O <sub>6</sub> Rb, HgN <sub>3</sub> O <sub>6</sub> Tl, Au <sub>6</sub> In <sub>5</sub> Na <sub>2</sub> ,
201	O <sub>9</sub> Sb <sub>3</sub> Tl <sub>2</sub> ,
204	P <sub>3</sub> Pd, Ge <sub>12</sub> Pt <sub>4</sub> Th, Ge <sub>12</sub> Pt <sub>4</sub> U, Ge <sub>12</sub> LaPt <sub>4</sub> , Al <sub>12</sub> Re, O <sub>3</sub> Re,
205	AlSb, AsGa, AsIn, AuSb <sub>2</sub> , AuN <sub>2</sub> , Bi <sub>2</sub> Pt, Bi <sub>2</sub> , N <sub>2</sub> Ta, NaO <sub>2</sub> , Cl <sub>4</sub> Pt, P <sub>2</sub> Pt <sub>6</sub> Sr, O <sub>2</sub> Pa, C <sub>2</sub> U, N <sub>2</sub> Re, As <sub>4</sub> Cl <sub>7</sub> Hg <sub>6</sub> Ti, As <sub>4</sub> Br <sub>7</sub> Hg <sub>6</sub> Ti, Cl <sub>7</sub> Hg <sub>6</sub> P <sub>4</sub> Ti,
206	C <sub>8</sub> , As <sub>2</sub> Zn <sub>3</sub> , Ge, Si, Bi <sub>2</sub> Mg <sub>3</sub> , Lu <sub>2</sub> N <sub>3</sub> , N <sub>3</sub> U <sub>2</sub> ,
208	Na <sub>11</sub> O <sub>16</sub> U <sub>5</sub> ,
210	O <sub>2</sub> Si,
212	BLi <sub>2</sub> Pd <sub>3</sub> , BLi <sub>2</sub> Pt <sub>3</sub> , Ga <sub>5</sub> LiO <sub>8</sub> , Si <sub>2</sub> Sr,
213	CaAl <sub>2</sub> Nb <sub>3</sub> , Au <sub>2</sub> Nb <sub>3</sub> , CaAl <sub>2</sub> Ta <sub>3</sub> , Al <sub>2</sub> NNb <sub>3</sub> , Mo <sub>3</sub> NPd <sub>2</sub> , Mo <sub>3</sub> NPt <sub>2</sub> , Ba <sub>24</sub> Ge <sub>100</sub> , Ag <sub>3</sub> AuS <sub>2</sub> , Ba <sub>24</sub> Si <sub>100</sub> , CMo <sub>3</sub> Re <sub>2</sub> , CRe <sub>2</sub> W <sub>3</sub> ,
214	C, Br <sub>3</sub> La <sub>3</sub> Si, I <sub>3</sub> La <sub>3</sub> Pb, GeI <sub>3</sub> La <sub>3</sub> , O <sub>9</sub> U <sub>4</sub> ,
215	Al <sub>3</sub> Li <sub>8</sub> Si <sub>5</sub> , C <sub>7</sub> B, Li <sub>10</sub> Pb <sub>3</sub> , Ag <sub>9</sub> In <sub>4</sub> , Ca <sub>4</sub> Hg <sub>9</sub> ,
216	AuBe <sub>5</sub> , AgAlLi <sub>2</sub> , AgAsMg, AgBiLi <sub>2</sub> , AgCdSb, AgLi <sub>2</sub> Pb, AgLi <sub>2</sub> Sn, AgMgSb, AgO, AgSe, Ag <sub>2</sub> LiSn,

Part 11 of all the predicted **Case 3-TSMs**:

	AlBi, AlLi <sub>2</sub> Pd, AlLi <sub>2</sub> Pt, AlTi <sub>2</sub> , AlTi <sub>2</sub> Zn, AsCdLi, AlTi <sub>3</sub> , AsIn, AsCsRb, AsTl, AuBiCa, AuBiLi <sub>2</sub> , AuCdSb, AlMo <sub>4</sub> S <sub>8</sub> , AuGeLi <sub>2</sub> , AuInLi <sub>2</sub> , AuLiSb, AuLiMgSn, AuLi <sub>2</sub> Pb, AuLi <sub>2</sub> Sn, AuMgSn,
216	AuN, AuPbY, BBi, BTi, Au <sub>5</sub> Ca, BiGa, BiIn, BiLiMg, BiPdY, CAg, CCd, CMo, CNSi, CNb, CPd, CSC, CTa, CW, CY, CdLi <sub>2</sub> Pb, CdN, CdPo, CdNa <sub>2</sub> Pb, CGaMo <sub>4</sub> S <sub>8</sub> , CsNRb, CsPRb, GaLi <sub>2</sub> Pd, GaLi <sub>2</sub> Pt, GaMo <sub>4</sub> Se <sub>4</sub> Te <sub>4</sub> , GaSb, GaMo <sub>4</sub> S <sub>8</sub> , GaMo <sub>4</sub> Se <sub>8</sub> , GaTi <sub>2</sub> , GaTi <sub>3</sub> , GaS <sub>8</sub> Ti <sub>4</sub> , GeInLi, GaNb <sub>4</sub> Se <sub>8</sub> , GeP, GeSc, HfN, GeTi <sub>3</sub> , GaMo <sub>4</sub> S <sub>8</sub> Si, HgSe, GaNb <sub>4</sub> S <sub>8</sub> , HgTe, InLi <sub>2</sub> Pd, InLi <sub>2</sub> Pt, InSb, InTi <sub>3</sub> , InTi <sub>2</sub> , GaSe <sub>8</sub> Ta <sub>4</sub> , LiMgPdSn, LiMgPdSb, LiMgPtSn, LiMgPtSb, GaSe <sub>4</sub> Ta <sub>4</sub> Te <sub>4</sub> , Li <sub>2</sub> PdSb, Li <sub>2</sub> PtSb, MgPtSb, MgPdSb, MoN, MoP, NPd, I <sub>4</sub> Nb <sub>4</sub> Se <sub>4</sub> , NPt, NTi, INbSe, Li <sub>2</sub> O <sub>4</sub> S, NW, NZn, NZr, PSi, PTl, PoZn, PtScSn, RbSb, RbTe, SbSn, SbTl, ScSn, SiTi <sub>3</sub> , SnTi <sub>3</sub> , Pd <sub>10</sub> Te <sub>3</sub> , AuSTa <sub>5</sub> , Mg <sub>5</sub> Pd <sub>10</sub> Si <sub>16</sub> , Mg <sub>5</sub> Pt <sub>10</sub> Si <sub>16</sub> , Ba <sub>14</sub> Li <sub>6</sub> N <sub>6</sub> Na <sub>10</sub> , Ba <sub>14</sub> Li <sub>5</sub> N <sub>6</sub> Na <sub>11</sub> , In <sub>2</sub> Te <sub>3</sub> , Li <sub>22</sub> Si <sub>5</sub> , Li <sub>17</sub> Pb <sub>4</sub> , BiLaPt, LuPtSb, AuPt <sub>4</sub> U, PaPt <sub>5</sub> , CRe, Cd <sub>45</sub> Lu <sub>11</sub> , Hg <sub>45</sub> La <sub>11</sub> , Li <sub>17</sub> Si <sub>4</sub> , Ge <sub>4</sub> Li <sub>17</sub> , AgLi <sub>2</sub> Sb,
217	Ag <sub>5</sub> Zn <sub>8</sub> , Ag <sub>5</sub> Cd <sub>8</sub> , Al <sub>12</sub> Mg <sub>17</sub> , Ge <sub>8</sub> Na <sub>6</sub> Pt <sub>8</sub> , Au <sub>5</sub> Cd <sub>8</sub> , Al <sub>12</sub> Ta <sub>17</sub> , Mg <sub>24</sub> Y <sub>5</sub> , K <sub>10</sub> Pb <sub>48</sub> , Pd <sub>16</sub> S <sub>7</sub> , OTa <sub>2</sub> , In <sub>5</sub> Na <sub>24</sub> O <sub>15</sub> , F <sub>9</sub> U <sub>2</sub> , Al <sub>5</sub> Re <sub>24</sub> , Re <sub>24</sub> Sc <sub>5</sub> , Re <sub>24</sub> Ti <sub>5</sub> , Mo <sub>5</sub> Re <sub>24</sub> , Re <sub>24</sub> Zr <sub>5</sub> , Hf <sub>5</sub> Re <sub>24</sub> , La <sub>6</sub> P <sub>17</sub> Pd <sub>6</sub> ,
218	Al <sub>6</sub> K <sub>8</sub> O <sub>24</sub> Si <sub>6</sub> , Al <sub>6</sub> Na <sub>8</sub> O <sub>24</sub> Si <sub>6</sub> ,
219	C <sub>4</sub> N <sub>4</sub> Tl <sub>2</sub> Zn,
220	Hf <sub>3</sub> N <sub>4</sub> , Li <sub>15</sub> Si <sub>4</sub> , Ge <sub>4</sub> Li <sub>15</sub> , Li <sub>12</sub> Mg <sub>3</sub> Si <sub>4</sub> , Li <sub>15</sub> Pd <sub>4</sub> , Na <sub>15</sub> Pb <sub>4</sub> , Na <sub>15</sub> Sn <sub>4</sub> , Ge <sub>3</sub> O <sub>12</sub> Sb <sub>4</sub> , O <sub>36</sub> P <sub>12</sub> Sc <sub>4</sub> , As <sub>3</sub> Ti <sub>4</sub> , Al <sub>3</sub> Li <sub>12</sub> Si <sub>4</sub> , Au <sub>3</sub> Sb <sub>4</sub> Y <sub>3</sub> , Ba <sub>4</sub> Bi <sub>3</sub> , Bi <sub>3</sub> Sr <sub>4</sub> , C <sub>3</sub> N <sub>4</sub> , C <sub>3</sub> Sc <sub>4</sub> , Cs <sub>4</sub> O <sub>6</sub> , N <sub>4</sub> Zr <sub>3</sub> , Ge <sub>3</sub> N <sub>4</sub> , P <sub>3</sub> Ti <sub>4</sub> , Sb <sub>3</sub> Y <sub>4</sub> , Au <sub>4</sub> Li <sub>15</sub> , C <sub>3</sub> Sc <sub>2</sub> , C <sub>3</sub> Y <sub>2</sub> , Bi <sub>4</sub> U <sub>3</sub> , Bi <sub>3</sub> La <sub>4</sub> , La <sub>4</sub> Pb <sub>3</sub> , P <sub>4</sub> Th <sub>3</sub> , Se <sub>4</sub> U <sub>3</sub> , P <sub>4</sub> U <sub>3</sub> , As <sub>4</sub> Pa <sub>3</sub> , La <sub>4</sub> Sb <sub>3</sub> , Au <sub>3</sub> Sn <sub>4</sub> U <sub>3</sub> , As <sub>4</sub> Th <sub>3</sub> , Pa <sub>3</sub> Sb <sub>4</sub> , La <sub>3</sub> Se <sub>4</sub> , Sb <sub>4</sub> U <sub>3</sub> , Pd <sub>3</sub> Sb <sub>4</sub> U <sub>3</sub> , Bi <sub>4</sub> Th <sub>3</sub> , As <sub>3</sub> La <sub>4</sub> , Ge <sub>3</sub> La <sub>4</sub> , Te <sub>4</sub> U <sub>3</sub> , Pt <sub>3</sub> Sb <sub>4</sub> U <sub>3</sub> , La <sub>3</sub> Te <sub>4</sub> , Sb <sub>4</sub> Th <sub>3</sub> , Pt <sub>3</sub> Sn <sub>4</sub> U <sub>3</sub> , Bi <sub>4</sub> La <sub>3</sub> Pt <sub>3</sub> , C <sub>3</sub> U <sub>2</sub> , C <sub>3</sub> Th <sub>2</sub> , C <sub>3</sub> Lu <sub>2</sub> , Ca <sub>12</sub> Li <sub>6</sub> N <sub>16</sub> O <sub>3</sub> Re <sub>4</sub> , P <sub>4</sub> Pa <sub>3</sub> , As <sub>4</sub> U <sub>3</sub> , Au <sub>3</sub> Lu <sub>3</sub> Sb <sub>4</sub> ,
221	AuCl <sub>3</sub> Cs, AuCa <sub>3</sub> N, CaIPt <sub>3</sub> , CInTi <sub>3</sub> , CW, CY, CSc <sub>3</sub> Tl, Cd <sub>3</sub> In, Ca <sub>3</sub> NPb, F <sub>3</sub> Ta, Ga <sub>3</sub> Sc, HfPt, InY, InPd <sub>3</sub> , CPt <sub>3</sub> Y, LiPb, BPt <sub>3</sub> Sc, F <sub>3</sub> Mo, MgPd <sub>3</sub> , PSc, InNSc <sub>3</sub> , CPbPt <sub>3</sub> , TiZn <sub>3</sub> , In <sub>3</sub> Sc, Pd <sub>3</sub> Sn, SnTi <sub>3</sub> , NaO <sub>3</sub> W, MoN, MgTl, MgY, NNb, NPd, NZr, NSc, NTi, NZn, NTa, NPd <sub>3</sub> , NbZn <sub>3</sub> , MoO <sub>3</sub> Sr, NNa <sub>3</sub> , Nb <sub>3</sub> Si, MgSc, NaPb <sub>3</sub> , NbO <sub>3</sub> Sr, P, MgSr, NbO, PY, PbPd <sub>3</sub> , N <sub>4</sub> W <sub>3</sub> , O <sub>3</sub> SnTa, PdSc, PdZr, Po, PdT <sub>i</sub> , PtSc, Pb <sub>3</sub> Y, Pd <sub>3</sub> Ti, Pd <sub>3</sub> Y, Pd <sub>3</sub> Zr, PtZr, PtTi, SbSn, Sb, STl, SbSc, SbTl, ScZn, SbY, Se, SeTl, SrTe, Pt <sub>3</sub> Ti, Pt <sub>3</sub> Zr, SrTl, Pt <sub>3</sub> Y, ZnZr, TiY, YZn, TiY, Sn <sub>3</sub> Y, Ti <sub>3</sub> Y, Pd <sub>17</sub> Se <sub>15</sub> , AgCd, AgMg, AgPt <sub>3</sub> , AgSc, AgY, AgZn, Ag <sub>3</sub> In, Ag <sub>3</sub> Mg, Ag <sub>3</sub> Pt, AlMo, AlPd, AlNTi <sub>3</sub> , AlPt <sub>3</sub> , AlZr <sub>3</sub> , AlY <sub>3</sub> , Al <sub>3</sub> Li, Al <sub>3</sub> Hf, Al <sub>3</sub> Ti, Al <sub>3</sub> Sc, Al <sub>3</sub> Zr, As, AsSc, AuCd, AsY, AuMg, AuPd <sub>3</sub> ,

Part 12 of all the predicted **Case 3-TSMs**:

	AuSc, AuTi, AuY, AuTi <sub>3</sub> , AuZn, Au <sub>3</sub> Li, Au <sub>3</sub> Pd, BPbSc <sub>3</sub> , BPd <sub>3</sub> Sc, BInSc <sub>3</sub> , BPd <sub>3</sub> Y, BSc <sub>3</sub> Sn, BSc <sub>3</sub> Tl, BPt <sub>3</sub> Y, B <sub>6</sub> K, BaCd, BaHg, BaNbO <sub>3</sub> , BaMoO <sub>3</sub> , B <sub>6</sub> Y, BaO <sub>3</sub> Pb, BaZn, BePd, Bi, BiTl, Bi <sub>3</sub> Sr, Br <sub>3</sub> CsHg, CaTi <sub>3</sub> , CaSc <sub>3</sub> , CCaPd <sub>3</sub> , CHf, CGaSc <sub>3</sub> , CGaY <sub>3</sub> , CInSc <sub>3</sub> , CNTl, CInPt <sub>3</sub> , CInY <sub>3</sub> , CNb, CMg <sub>3</sub> Zn, CPbSc <sub>3</sub> , CPbY <sub>3</sub> , Cpt, CPd <sub>3</sub> Y, CSc, CPd <sub>3</sub> Sc, CPt <sub>3</sub> Sc, CSnY <sub>3</sub> , CTa, CSc <sub>3</sub> Sn, CZr, CTIY <sub>3</sub> , CTi <sub>3</sub> Tl, Ca, CaCd, CaHg, CaIn, CaPb <sub>3</sub> , CaTe, CaSn <sub>3</sub> , CaTl, CaTl <sub>3</sub> , Ca <sub>3</sub> NSn, Ca <sub>3</sub> NTl, Ca <sub>3</sub> Pb, CdN, CdSr, CdY, CdSc, Cd <sub>3</sub> Nb, C <sub>20</sub> , CsNO <sub>2</sub> , CsIO <sub>3</sub> , F <sub>3</sub> KPd, F <sub>3</sub> PdRb, F <sub>3</sub> Nb, GaPt <sub>3</sub> , GeNb <sub>3</sub> , GeTe, HfPd, HfPt <sub>3</sub> , Al <sub>2</sub> Ca <sub>3</sub> O <sub>6</sub> , HgLi, HgSc, HgSr, HgTl, HgY, Hg <sub>3</sub> Zr, Hg <sub>3</sub> Tl, InPd, InMg <sub>3</sub> , InSb, InPt <sub>3</sub> , InNTi <sub>3</sub> , InSc <sub>3</sub> , InTe, InZr <sub>3</sub> , In <sub>3</sub> Mg, In <sub>3</sub> Y, LiPd, CaHg <sub>11</sub> , BaHg <sub>11</sub> , Hg <sub>11</sub> K, In <sub>14</sub> K <sub>3</sub> Mg <sub>20</sub> , Hg <sub>11</sub> Rb, Hg <sub>11</sub> Sr, BiMg <sub>64</sub> Si <sub>31</sub> , AgLa, AsTh, AsU, AuLu, AlLu <sub>3</sub> N, BInLa <sub>3</sub> , BLuPd <sub>3</sub> , ALLa <sub>3</sub> , BLaPd <sub>3</sub> , B <sub>6</sub> La, ALLa <sub>3</sub> N, BLaPt <sub>3</sub> , BiTh, BiU, Ga <sub>3</sub> U, CdLu, CLa <sub>3</sub> Tl, InLa, HgLa, HgLu, In <sub>3</sub> Lu, LaZn, Ga <sub>3</sub> Lu, GaLaO <sub>3</sub> , LuPd, LuPd <sub>3</sub> , LuMg, LaTl, LuSb, LuPt <sub>3</sub> , KO <sub>3</sub> U, LuPb <sub>3</sub> , LaTe, B <sub>6</sub> Th, LuTl <sub>3</sub> , In <sub>3</sub> La, LaPd <sub>3</sub> , O <sub>3</sub> RbU, LaPb <sub>3</sub> , LaPt <sub>3</sub> , InLa <sub>3</sub> , SbU, SbTh, TeTh, LaO <sub>3</sub> Ti, In <sub>3</sub> U, ThTl <sub>3</sub> , La <sub>3</sub> Tl, LaSn <sub>3</sub> , La <sub>3</sub> Sn, Si <sub>3</sub> U, TeU, LaTl <sub>3</sub> , CLaPd <sub>3</sub> , InLa <sub>3</sub> N, Tl <sub>3</sub> U, Pb <sub>3</sub> Th, CAI <sub>3</sub> , CLa <sub>3</sub> Pb, InLu <sub>3</sub> N, CLaPt <sub>3</sub> , B <sub>6</sub> Lu, CLu <sub>3</sub> Sn, S <sub>3</sub> U <sub>4</sub> , Cd <sub>11</sub> La, Cd <sub>11</sub> Th, AlRe, CRe, NRe, ReTi, O <sub>3</sub> Re, PbTi,
221	AlMo <sub>3</sub> , AlNb <sub>3</sub> , AsTi <sub>3</sub> , AuTl <sub>3</sub> , AuTi <sub>3</sub> , AuNb <sub>3</sub> , AuTa <sub>3</sub> , AuZr <sub>3</sub> , BeMo <sub>3</sub> , Cl <sub>3</sub> Na, GaMo <sub>3</sub> , GaNb <sub>3</sub> , CaO <sub>4</sub> Pd <sub>3</sub> , CdO <sub>4</sub> Pd <sub>3</sub> , GeMo <sub>3</sub> , GeNb <sub>3</sub> , AuZn <sub>3</sub> , Ba <sub>2</sub> Si <sub>46</sub> , Ba <sub>6</sub> Si <sub>46</sub> , Ba <sub>6</sub> Na <sub>2</sub> Si <sub>46</sub> , InNb <sub>3</sub> , Ba <sub>8</sub> Si <sub>46</sub> , Mo <sub>3</sub> Pt, Mo <sub>3</sub> Si, NPd <sub>3</sub> , Mo <sub>3</sub> Sn, NaO <sub>4</sub> Pd <sub>3</sub> , Cs <sub>3</sub> Hg <sub>20</sub> , NaO <sub>4</sub> Pt <sub>3</sub> , Nb <sub>3</sub> Pb, Nb <sub>3</sub> Pt, Ga <sub>16</sub> Ge <sub>30</sub> Na <sub>8</sub> , Nb <sub>3</sub> Sn, Nb <sub>3</sub> Si, Hg <sub>20</sub> Rb <sub>3</sub> , Nb <sub>3</sub> Te, Nb <sub>3</sub> Tl, OW <sub>3</sub> , OW <sub>3</sub> , Ge <sub>30</sub> In <sub>16</sub> K <sub>8</sub> , O <sub>4</sub> Pd <sub>3</sub> Sr, K <sub>8</sub> Si <sub>46</sub> , O <sub>4</sub> Pt <sub>3</sub> , Ge <sub>40</sub> In <sub>6</sub> K <sub>8</sub> , PdT <sub>3</sub> , PtTi <sub>3</sub> , PtTl <sub>3</sub> , Au <sub>6</sub> Ba <sub>8</sub> Ge <sub>40</sub> , Pd <sub>3</sub> S <sub>4</sub> Y, SbTi <sub>3</sub> , SnTa <sub>3</sub> , Ba <sub>4</sub> Ge <sub>20</sub> Pd <sub>3</sub> , SnZr <sub>3</sub> , Au <sub>6</sub> Ba <sub>8</sub> Si <sub>40</sub> , Ag <sub>3</sub> Ba <sub>4</sub> Ge <sub>20</sub> , Au <sub>3</sub> Ba <sub>4</sub> Ge <sub>20</sub> , Na <sub>4</sub> Si <sub>23</sub> , Ge <sub>46</sub> K <sub>8</sub> , Na <sub>8</sub> Si <sub>46</sub> , Ba <sub>4</sub> Ge <sub>20</sub> Pt <sub>3</sub> , Cs <sub>8</sub> Sn <sub>46</sub> , Cs <sub>4</sub> Sn <sub>23</sub> , Cs <sub>4</sub> Sn <sub>23</sub> , K <sub>8</sub> Sn <sub>46</sub> , In <sub>48</sub> K <sub>3</sub> Na <sub>26</sub> , In <sub>48</sub> Na <sub>26</sub> Rb <sub>3</sub> , LaPd <sub>3</sub> S <sub>4</sub> ,
224	OPb <sub>2</sub> , Ag <sub>2</sub> O, Ag <sub>2</sub> O <sub>3</sub> , Bi <sub>2</sub> O <sub>3</sub> , OPd <sub>2</sub> , OZr <sub>2</sub> , O <sub>2</sub> Pt,
225	Br, NbO, O <sub>2</sub> Pb, RbSb, Pt <sub>7</sub> Sb, Ga <sub>16</sub> Pd <sub>7</sub> Zr <sub>6</sub> , Al <sub>4</sub> Sn <sub>3</sub> Sr <sub>11</sub> , Mg <sub>23</sub> Sr <sub>6</sub> , Hf, HgPo, GeLi <sub>2</sub> Zn, LiS, Li, InSb, HgTe, HgSe, K, In <sub>2</sub> LiPd, InPd <sub>2</sub> Y, HgLi <sub>3</sub> , KN, InPt <sub>2</sub> Sc, InPt <sub>2</sub> Zr, LiPd <sub>2</sub> Sn, LiPbPd <sub>2</sub> , KS, InTe, Mo, Li <sub>2</sub> MgPb, InSr <sub>3</sub> , LiMg <sub>2</sub> Si, MoN, Mg <sub>2</sub> Pb, Sb, SY, InP, TeY, SZr, Ti, In <sub>2</sub> Pt, Zr, Li <sub>3</sub> Pd, PSn, Pd, Si, MoP, Y, Sc, Pt, Nb, OZr, NZn, NZr, NTi, NNb, Ta, PZr, NPd, Li <sub>2</sub> SnZn, OTi, NNa, MgP <sub>2</sub> Si, NaS, OTa, Rf, NW,

Part 13 of all the predicted **Case 3-TSMs**:

225	Li <sub>3</sub> Tl, Li <sub>2</sub> MgTl, NTa, OPt, NPt, SSc, In <sub>2</sub> LiPt, PoY, ScSe, LiPd <sub>7</sub> , SbSn, SeY, P <sub>2</sub> SiZn, NPd <sub>3</sub> , InLi <sub>2</sub> Mg, Pd <sub>2</sub> ScSn, Pd <sub>2</sub> SnY, PbPd <sub>2</sub> Y, RbTe, Pt <sub>2</sub> ScSn, INaO <sub>6</sub> Pb <sub>2</sub> , LiPt <sub>7</sub> , MoZn <sub>6</sub> , MoZn <sub>7</sub> , Li <sub>23</sub> Sr <sub>6</sub> , In <sub>8</sub> N <sub>7</sub> Sr <sub>19</sub> , AgAuCd <sub>2</sub> , AgAuZn <sub>2</sub> , AgAuCl <sub>6</sub> Cs <sub>2</sub> , AgCs <sub>2</sub> F <sub>6</sub> K, AgN, Ag <sub>2</sub> AlSc, Ag <sub>2</sub> CdMg, Ag <sub>2</sub> GeLi, Ag <sub>2</sub> InLi, Ag <sub>2</sub> InMg, Ag <sub>2</sub> InSc, Ag <sub>2</sub> InY, Ag <sub>2</sub> LiSn, Al <sub>16</sub> Hf <sub>6</sub> Pt <sub>7</sub> , AlAu <sub>2</sub> Hf, AlAu <sub>2</sub> Ti, AlTiZr <sub>2</sub> , Al <sub>2</sub> Au, Al <sub>2</sub> LiPt, Al <sub>2</sub> Pt, AsIn, AsSn, AsTe, AsZr, AuGa <sub>2</sub> , AuIn <sub>2</sub> , AuN, Au <sub>2</sub> HfIn, Au <sub>2</sub> InTi, Au <sub>2</sub> InZr, B <sub>12</sub> Sc, Al <sub>16</sub> Pt <sub>7</sub> Ti <sub>6</sub> , B <sub>12</sub> Y, B <sub>12</sub> Zr, BBe <sub>2</sub> , BZr, Ba <sub>2</sub> CaO <sub>6</sub> Re, Ba <sub>2</sub> CdO <sub>6</sub> Re, Ag <sub>8</sub> Ca <sub>19</sub> N <sub>7</sub> , Ba <sub>2</sub> O <sub>6</sub> SbSc, Ba <sub>2</sub> O <sub>6</sub> ReY, Ba <sub>2</sub> O <sub>6</sub> ReZn, BeP <sub>2</sub> Si, Be <sub>2</sub> Si, BiK <sub>3</sub> , BiO <sub>2</sub> , BiSe, BiTe, Br <sub>6</sub> Cs <sub>2</sub> W, Br <sub>6</sub> K <sub>2</sub> Re, Ba <sub>6</sub> Mg <sub>23</sub> , CAg, CCd, CMo, CNb, CSc, CTi, CRe, CTa, CY, Br <sub>6</sub> Rb <sub>2</sub> W, Ca <sub>3</sub> In, Ca <sub>3</sub> Tl, Ca <sub>2</sub> O <sub>6</sub> PdW, Ca <sub>6</sub> GeLi, CdGeLi <sub>2</sub> , CdGeP <sub>2</sub> , CdLi <sub>2</sub> Pb, CdN, CdP <sub>2</sub> Si, Cd <sub>3</sub> Y, Cl <sub>6</sub> Cs <sub>2</sub> Mo, Cl <sub>6</sub> Cs <sub>2</sub> Re, Cl <sub>6</sub> Cs <sub>2</sub> Ta, Cl <sub>6</sub> Cs <sub>2</sub> W, Cl <sub>6</sub> K <sub>2</sub> Mo, Cl <sub>6</sub> K <sub>2</sub> Re, Cl <sub>6</sub> K <sub>2</sub> Ta, Cl <sub>6</sub> MoTl <sub>2</sub> , Cl <sub>6</sub> NbRb <sub>2</sub> , Cl <sub>6</sub> K <sub>2</sub> W, Cs, Cl <sub>6</sub> Rb <sub>2</sub> W, Cl <sub>6</sub> Tl <sub>2</sub> W, Cs <sub>2</sub> F <sub>6</sub> KMo, Cs <sub>2</sub> F <sub>6</sub> KTi, Cs <sub>2</sub> F <sub>6</sub> MoTl, Ca <sub>19</sub> In <sub>8</sub> N <sub>7</sub> , F <sub>2</sub> Ti, F <sub>6</sub> KMoRb <sub>2</sub> , F <sub>6</sub> K <sub>2</sub> MoNa, F <sub>6</sub> KMoTl <sub>2</sub> , F <sub>6</sub> KRb <sub>2</sub> Ti, F <sub>6</sub> MoNaRb <sub>2</sub> , F <sub>6</sub> K <sub>3</sub> Mo, F <sub>6</sub> MoNa, F <sub>6</sub> MoNaTl <sub>2</sub> , F <sub>6</sub> NaRb <sub>2</sub> Ti, F <sub>6</sub> K <sub>3</sub> W, F <sub>6</sub> TiTl <sub>3</sub> , F <sub>6</sub> TiZr, Ga <sub>2</sub> LiPd, GaPd <sub>2</sub> Sc, Ga <sub>2</sub> Pt, Ga <sub>2</sub> LiPt, GeLiMg <sub>2</sub> , GeLiPd <sub>2</sub> , GeLi <sub>2</sub> Pd, GeHgLi <sub>2</sub> , Ga <sub>16</sub> Hf <sub>6</sub> Pd <sub>7</sub> , Ga <sub>16</sub> Pt <sub>7</sub> Zr <sub>6</sub> , Ga <sub>16</sub> Pt <sub>7</sub> Ti <sub>6</sub> , Ga <sub>4</sub> Sn <sub>3</sub> Sr <sub>11</sub> , BBr <sub>20</sub> K <sub>8</sub> Zr <sub>6</sub> , Ac, AsPa, AsTh, Au <sub>2</sub> InU, AsU, Au <sub>2</sub> SnU, Au <sub>2</sub> InTh, Ag <sub>2</sub> InLa, CPa, CU, CTh, C <sub>2</sub> U, OU, OPa, NU, PTh, La, NTh, LaN, SeTh, LaS, PU, LuSe, LuS, LaSe, LuTe, Th, LuPo, InLuPd <sub>2</sub> , LuPd <sub>2</sub> Sn, SbTh, SbU, LaMg <sub>3</sub> , B <sub>12</sub> Lu, Cl <sub>6</sub> Cs <sub>2</sub> NaU, Lu <sub>6</sub> Zn <sub>23</sub> , AlLa <sub>6</sub> Mg <sub>22</sub> , Mg <sub>23</sub> Th <sub>6</sub> , Cd <sub>23</sub> Th <sub>6</sub> , NRe, Re, Ba <sub>2</sub> MgO <sub>6</sub> Re, Pt <sub>23</sub> Si <sub>11</sub> U <sub>3</sub> , U,
226	Be <sub>13</sub> Sr, Be <sub>13</sub> Sb, Be <sub>13</sub> Sc, BaBe <sub>13</sub> , CaZn <sub>13</sub> , Be <sub>13</sub> Ca, Be <sub>13</sub> Zr, Be <sub>13</sub> Hf, LiZn <sub>13</sub> , Be <sub>13</sub> Y, KZn <sub>13</sub> , NaZn <sub>13</sub> , RbZn <sub>13</sub> , BaZn <sub>13</sub> , BeZn <sub>13</sub> , Cd <sub>13</sub> Cs, Cd <sub>13</sub> K, SrZn <sub>13</sub> , Mo <sub>7</sub> Sn <sub>12</sub> Zn <sub>40</sub> , Be <sub>13</sub> Lu, Be <sub>13</sub> La, Be <sub>13</sub> Th, LaZn <sub>13</sub> , Cd <sub>13</sub> Rb,
227	Ca <sub>2</sub> FO <sub>6</sub> Ta <sub>2</sub> , NZn <sub>3</sub> Zr <sub>3</sub> , NTi <sub>3</sub> Zn <sub>3</sub> , AgBe <sub>2</sub> , Ag <sub>2</sub> Na, Be <sub>2</sub> Nb, B <sub>2</sub> Sc, Au <sub>2</sub> Na, Al <sub>2</sub> Sc, CaPd <sub>2</sub> , CaLi <sub>2</sub> , Be <sub>2</sub> Ta, CaPt <sub>2</sub> , Al <sub>2</sub> Y, Bi <sub>2</sub> Rb, BaPd <sub>2</sub> , As <sub>2</sub> Na, Au <sub>2</sub> Pb, Au <sub>2</sub> Bi, BaPt <sub>2</sub> , Bi <sub>2</sub> K, Bi <sub>2</sub> Cs, Ge, AgIn <sub>2</sub> Na <sub>3</sub> , LiZn, InLi, HfW <sub>2</sub> , InNa, Mo <sub>2</sub> Zr, LiPt <sub>2</sub> , HfMo <sub>2</sub> , CsO <sub>6</sub> W <sub>2</sub> , NaPt <sub>2</sub> , In <sub>24</sub> S <sub>32</sub> , BiF <sub>4</sub> K, Pd <sub>2</sub> Sr, Pt <sub>2</sub> Sr, O <sub>4</sub> PdZn <sub>2</sub> , Sn, Pt <sub>2</sub> Y, YZn <sub>2</sub> , LiO <sub>4</sub> Ti <sub>2</sub> , W <sub>2</sub> Zr, PdSc <sub>2</sub> , O <sub>7</sub> Pb <sub>2</sub> Sb <sub>2</sub> , S <sub>4</sub> Zr <sub>3</sub> , ILi <sub>7</sub> N <sub>2</sub> , O <sub>6</sub> Pb <sub>2</sub> Sn <sub>2</sub> , NNb <sub>3</sub> Zn <sub>3</sub> , NaO <sub>3</sub> Sb, AlMg <sub>3</sub> Pt <sub>2</sub> , Hf <sub>2</sub> Pt, AuIn <sub>2</sub> Na <sub>3</sub> , O <sub>4</sub> Sb <sub>2</sub> , O <sub>5</sub> Sb <sub>2</sub> , OPd <sub>2</sub> Zr <sub>4</sub> , HfZn <sub>22</sub> , PtZr <sub>2</sub> , AsPd <sub>5</sub> Sb, Ge <sub>136</sub> K <sub>24</sub> , CZn <sub>3</sub> Zr <sub>3</sub> , Al <sub>18</sub> Mg <sub>3</sub> Ta <sub>2</sub> , CHf <sub>3</sub> Zn <sub>3</sub> , Zn <sub>22</sub> Zr, BMg <sub>8</sub> Pt <sub>4</sub> , Ba <sub>10</sub> Ga, LuS <sub>2</sub> , Al <sub>2</sub> U, Al <sub>2</sub> Lu, Al <sub>2</sub> La, LaPt <sub>2</sub> , LaMg <sub>2</sub> , Cs <sub>2</sub> O <sub>12</sub> U <sub>4</sub> , Be <sub>22</sub> Re, Al <sub>2</sub> BRe <sub>3</sub> , NRe <sub>2</sub> Zr <sub>4</sub> , Al <sub>20</sub> LaTi <sub>2</sub> , CTi <sub>3</sub> Zn <sub>3</sub> , CsGe <sub>17</sub> Na <sub>2</sub> , CdLi, Na <sub>2</sub> RbSi <sub>17</sub> ,
229	Se, W, Al, Ba, Ca, Bi, AuSb <sub>3</sub> , Cs, Hf, Mg, Li, Mo, K, Na, Nb, Rb, Sb, Sn, Ti, Ta, Sr, Tl, Zr, Ca <sub>5</sub> Ge <sub>6</sub> Pd <sub>6</sub> , Ag <sub>8</sub> Ca <sub>3</sub> , O <sub>4</sub> Pt <sub>3</sub> , F <sub>15</sub> Nb <sub>6</sub> , In <sub>7</sub> Pt <sub>3</sub> , Ga <sub>12</sub> PtY <sub>4</sub> , Ga <sub>7</sub> Pd <sub>3</sub> , Al <sub>14</sub> Mg <sub>13</sub> , In <sub>7</sub> Pd <sub>3</sub> , Ga <sub>7</sub> Pt <sub>3</sub> ,

Part 14 of all the predicted **Case 3-TSMs**:

<b>229</b>	Sb <sub>2</sub> Tl <sub>7</sub> , Mo <sub>3</sub> Sb <sub>7</sub> , Ca <sub>17</sub> Hg <sub>9</sub> Li <sub>6</sub> , La, Th, Lu, Cd <sub>4</sub> La <sub>6</sub> Pd <sub>13</sub> , Ga <sub>12</sub> Lu <sub>4</sub> Pd, Ga <sub>12</sub> PdU <sub>4</sub> , La <sub>6</sub> Pd <sub>13</sub> Zn <sub>4</sub> , K <sub>4</sub> O <sub>12</sub> SrU <sub>3</sub> , As <sub>7</sub> Re <sub>3</sub> , U,
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Note that materials in **Cases 1** and **2** can also have band crossings located near the Fermi energy. We list the potential materials with such properties in the following table. Blue and red colors respectively denote **Cases 1** and **2**.

Part 1 of all the predicted materials with band crossings from **Cases 1 or 2**:

TABLE VIII. Materials with band crossings in **Cases 1 or 2** (in blue or red, respectively): The band crossings for the materials listed here could be far from the Fermi energy, and the material might have a continuous direct gap or even a full band gap. One must further examine the actual band dispersions in understanding the prospect of these materials as TSM candidates.

<i>Sg</i>	Materials
<b>1</b>	AlCl <sub>7</sub> Se, Al <sub>2</sub> Li <sub>2</sub> O <sub>12</sub> Si <sub>4</sub> , Al <sub>2</sub> O <sub>4</sub> Pb, AsKSe <sub>2</sub> , Au <sub>2</sub> Te <sub>3</sub> , B <sub>2</sub> Cd <sub>2</sub> O <sub>5</sub> , B <sub>3</sub> BiO <sub>6</sub> , BaBeFO <sub>4</sub> P, BaF <sub>12</sub> Sb <sub>2</sub> , BaI <sub>4</sub> O <sub>12</sub> Pd, BeP <sub>2</sub> , C, CLiNaO <sub>3</sub> , CaGe <sub>2</sub> O <sub>5</sub> , Ca <sub>8</sub> In <sub>3</sub> , Cl <sub>4</sub> Cs <sub>2</sub> Hg, Cl <sub>7</sub> N <sub>2</sub> SbSe <sub>3</sub> , Cs <sub>10</sub> K <sub>6</sub> Pb <sub>36</sub> , Cs <sub>4</sub> Mo <sub>3</sub> O <sub>20</sub> U <sub>3</sub> , F <sub>4</sub> NO <sub>3</sub> RbTe, F <sub>6</sub> Na <sub>2</sub> Si, F <sub>6</sub> Na <sub>2</sub> Ti, Ga <sub>2</sub> O <sub>11</sub> Te <sub>4</sub> , Ga <sub>2</sub> O <sub>4</sub> Pb, IKO <sub>3</sub> , KSbSe <sub>2</sub> , LiN <sub>2</sub> Na <sub>5</sub> , O <sub>11</sub> Sr <sub>3</sub> Te <sub>4</sub> , O <sub>2</sub> Si, O <sub>2</sub> Ti, O <sub>6</sub> Sb <sub>2</sub> W, O <sub>8</sub> Se <sub>2</sub> Te <sub>2</sub> , P <sub>2</sub> PtSi <sub>3</sub> , Pb <sub>4</sub> S <sub>13</sub> Sb <sub>6</sub> , RbS <sub>2</sub> Sb, RbSbSe <sub>2</sub> , S <sub>4</sub> SbTl <sub>3</sub> ,
<b>2</b>	Si <sub>2</sub> Te <sub>6</sub> Tl <sub>6</sub> ,
<b>3</b>	GeO <sub>5</sub> Pb <sub>3</sub> , O <sub>2</sub> Si,
<b>4</b>	Ag <sub>2</sub> S, AlBaF <sub>5</sub> , AlCl <sub>4</sub> K, AlCl <sub>6</sub> I, Al <sub>2</sub> O <sub>12</sub> W <sub>3</sub> , Al <sub>2</sub> O <sub>4</sub> Sr, Al <sub>7</sub> S <sub>12</sub> Tl <sub>3</sub> , AsCsF <sub>4</sub> , AsF <sub>12</sub> LiXe <sub>3</sub> , AsLiMoO <sub>6</sub> , AsO <sub>4</sub> TlZn, AsS <sub>2</sub> , As <sub>2</sub> Ba <sub>2</sub> Se <sub>5</sub> , As <sub>2</sub> CdHg <sub>4</sub> I <sub>4</sub> , As <sub>2</sub> Cs <sub>2</sub> Se <sub>9</sub> Sn, As <sub>2</sub> K <sub>3</sub> LaO <sub>8</sub> , As <sub>2</sub> O <sub>3</sub> , As <sub>2</sub> Pb <sub>2</sub> S <sub>5</sub> , As <sub>8</sub> Pb <sub>8</sub> S <sub>20</sub> , AuBr <sub>6</sub> , AuNa <sub>5</sub> Se <sub>12</sub> , B <sub>4</sub> GeO <sub>9</sub> Rb <sub>2</sub> , BaMo <sub>2</sub> O <sub>9</sub> Te, BaMo <sub>3</sub> O <sub>10</sub> , BaNa <sub>2</sub> O <sub>6</sub> Si <sub>2</sub> , BaO <sub>9</sub> TeW <sub>2</sub> , Ba <sub>2</sub> Cl <sub>7</sub> Sc, Ba <sub>3</sub> P <sub>4</sub> Sn <sub>2</sub> , BiCl <sub>5</sub> Hg <sub>4</sub> S <sub>2</sub> , BiInS <sub>3</sub> , BiKP <sub>2</sub> S <sub>6</sub> , BiKP <sub>2</sub> Se <sub>6</sub> , BiP <sub>2</sub> S <sub>6</sub> Tl, BiPd, Bi <sub>4</sub> Br <sub>2</sub> O <sub>5</sub> , Bi <sub>4</sub> I <sub>2</sub> O <sub>5</sub> , Br <sub>10</sub> Re <sub>2</sub> Te <sub>6</sub> , Br <sub>4</sub> K <sub>2</sub> Zn, C <sub>2</sub> F <sub>4</sub> Te <sub>2</sub> , C <sub>2</sub> N <sub>2</sub> S <sub>9</sub> , CaGe <sub>2</sub> Pt <sub>2</sub> , CaN <sub>2</sub> O <sub>2</sub> Si <sub>2</sub> , CaO <sub>3</sub> Te, Ca <sub>2</sub> Nb <sub>2</sub> O <sub>7</sub> , Ca <sub>4</sub> FNa <sub>2</sub> NbO <sub>17</sub> Si <sub>4</sub> Zr, Cd <sub>2</sub> O <sub>12</sub> Rb <sub>2</sub> S <sub>3</sub> , ClFO <sub>7</sub> Pb <sub>2</sub> Se <sub>2</sub> Ti, ClHg <sub>2</sub> O <sub>12</sub> Rb <sub>3</sub> S <sub>3</sub> , ClHg <sub>2</sub> O <sub>12</sub> S <sub>3</sub> Tl <sub>3</sub> , ClNbO <sub>8</sub> Pb <sub>2</sub> Se <sub>2</sub> , Cl <sub>2</sub> N <sub>2</sub> S <sub>3</sub> , Cl <sub>9</sub> Hg <sub>6</sub> In <sub>2</sub> P <sub>3</sub> , Cs <sub>2</sub> HgI <sub>4</sub> , Cs <sub>4</sub> O <sub>3</sub> Pb, F <sub>12</sub> Sb <sub>2</sub> Xe, F <sub>21</sub> Rb <sub>5</sub> Zr <sub>4</sub> , F <sub>2</sub> OTe, F <sub>3</sub> KOTe, F <sub>7</sub> SnY, GeKS <sub>4</sub> Y, GeN <sub>2</sub> OSi, GeO <sub>5</sub> Pb <sub>3</sub> , HfNO <sub>3</sub> Ta, HgI <sub>2</sub> O <sub>6</sub> , Hg <sub>3</sub> O <sub>10</sub> SeTe <sub>2</sub> , Hg <sub>3</sub> O <sub>10</sub> Se <sub>3</sub> , ILiMoO <sub>6</sub> , I <sub>4</sub> O <sub>12</sub> Zn <sub>2</sub> , I <sub>4</sub> Tl <sub>2</sub> Zn, InK <sub>2</sub> LiMo <sub>3</sub> O <sub>12</sub> , InP <sub>2</sub> S <sub>6</sub> Tl, In <sub>6</sub> Se <sub>7</sub> , KLiO <sub>5</sub> Si <sub>2</sub> , KP <sub>2</sub> S <sub>6</sub> Sb, KP <sub>2</sub> SbSe <sub>6</sub> , KS <sub>4</sub> SiY, K <sub>2</sub> Mo <sub>3</sub> Se <sub>18</sub> , K <sub>2</sub> O <sub>15</sub> Si <sub>6</sub> Ti, MoO <sub>2</sub> , MoO <sub>7</sub> TeZn <sub>2</sub> , NaP <sub>2</sub> S <sub>6</sub> Sb, Na <sub>2</sub> O <sub>8</sub> Si <sub>3</sub> Zn, Na <sub>2</sub> Se <sub>9</sub> Ti <sub>2</sub> , O <sub>11</sub> P <sub>2</sub> W <sub>2</sub> , O <sub>15</sub> Pb <sub>4</sub> SSi <sub>3</sub> Zn <sub>2</sub> , O <sub>5</sub> Te <sub>2</sub> , P <sub>2</sub> PtSi <sub>2</sub> , P <sub>2</sub> S <sub>6</sub> SbTl, P <sub>2</sub> SbSe <sub>6</sub> Tl, P <sub>2</sub> Se <sub>6</sub> TlY, P <sub>4</sub> S <sub>5</sub> , SbSe <sub>2</sub> Tl, Se, Te,
<b>5</b>	AgS <sub>2</sub> Sb, Ag <sub>2</sub> Mo <sub>3</sub> O <sub>16</sub> Te <sub>3</sub> , Al <sub>17</sub> Mo <sub>4</sub> , AlAs <sub>2</sub> LiO <sub>7</sub> , Al <sub>4</sub> O <sub>15</sub> Sr <sub>6</sub> Y <sub>2</sub> , Al <sub>4</sub> P <sub>6</sub> S <sub>18</sub> , Al <sub>6</sub> F <sub>21</sub> NaRb <sub>2</sub> , AsPd <sub>5</sub> , As <sub>2</sub> GaLiO <sub>7</sub> , As <sub>2</sub> LiO <sub>7</sub> Sc, As <sub>2</sub> Mo, As <sub>2</sub> NaO <sub>7</sub> Sc, As <sub>2</sub> Nb, As <sub>2</sub> Ta, AuCsI <sub>4</sub> O <sub>12</sub> , AuI <sub>4</sub> KO <sub>12</sub> , AuI <sub>4</sub> O <sub>12</sub> Rb, BBe <sub>2</sub> FO <sub>3</sub> , BBe <sub>2</sub> F <sub>2</sub> KO <sub>3</sub> , BBe <sub>2</sub> F <sub>2</sub> O <sub>3</sub> Rb, B <sub>3</sub> BiO <sub>6</sub> , Bi <sub>10</sub> Mo <sub>3</sub> O <sub>24</sub> , Bi <sub>14</sub> Mo <sub>5</sub> O <sub>36</sub> , BiO <sub>3</sub> Sc, Bi <sub>7</sub> F <sub>11</sub> O <sub>5</sub> , BrHg <sub>3</sub> ITe <sub>2</sub> , Br <sub>2</sub> NbO, Br <sub>4</sub> NbOTl, CCaO <sub>3</sub> , CK <sub>4</sub> O <sub>4</sub> , CLi <sub>4</sub> O <sub>4</sub> , CNa <sub>4</sub> O <sub>4</sub> , C <sub>3</sub> AsN <sub>3</sub> , CaO <sub>7</sub> Si <sub>2</sub> Zr, CdNa <sub>2</sub> S <sub>4</sub> Sn, GaNbO <sub>4</sub> , Ga <sub>2</sub> Ge <sub>3</sub> O <sub>10</sub> Rb <sub>2</sub> , GePd <sub>5</sub> , Ge <sub>2</sub> Hg <sub>3</sub> K <sub>2</sub> S <sub>8</sub> , Ge <sub>4</sub> O <sub>9</sub> Pb, Ge <sub>9</sub> Li <sub>4</sub> O <sub>20</sub> , Hg <sub>2</sub> P <sub>2</sub> S <sub>7</sub> , I <sub>2</sub> NbO, I <sub>3</sub> NbO, InKP <sub>2</sub> S <sub>7</sub> , LiN <sub>2</sub> Na <sub>5</sub> , MoO <sub>4</sub> Tl <sub>2</sub> , Mo <sub>3</sub> Na <sub>2</sub> O <sub>16</sub> Te <sub>3</sub> , Na <sub>4</sub> O <sub>9</sub> Si <sub>3</sub> Sr, Nb <sub>2</sub> O <sub>5</sub> , O <sub>14</sub> PtSi <sub>2</sub> Sr <sub>8</sub> , O <sub>2</sub> Si, O <sub>5</sub> Ta <sub>2</sub> , P <sub>2</sub> S <sub>7</sub> ScTl, PbS, Pb <sub>3</sub> Pd <sub>5</sub> , Po, Re <sub>2</sub> Sc <sub>3</sub> Si <sub>3</sub> ,
<b>6</b>	BO <sub>3</sub> Y, BaBe <sub>2</sub> O <sub>7</sub> Si <sub>2</sub> , CGa <sub>3</sub> N <sub>3</sub> Si, C <sub>3</sub> GaNSi <sub>3</sub> , CsIO <sub>3</sub> , CsI <sub>4</sub> Li <sub>3</sub> , Li <sub>3</sub> N <sub>2</sub> Na <sub>3</sub> , Li <sub>5</sub> N <sub>2</sub> Na, NO <sub>2</sub> SiY, NbSe <sub>3</sub> , O <sub>2</sub> Si,
<b>7</b>	Ag <sub>7</sub> S <sub>6</sub> Ta, CLi <sub>4</sub> O <sub>4</sub> , Ca <sub>14</sub> F <sub>2</sub> Nb <sub>2</sub> O <sub>34</sub> Si <sub>8</sub> , HgO <sub>4</sub> S, O <sub>3</sub> W,
<b>8</b>	B <sub>3</sub> Ca <sub>4</sub> LaO <sub>10</sub> , N <sub>2</sub> Re,
<b>9</b>	Al <sub>15</sub> La <sub>3</sub> O <sub>37</sub> Ti <sub>5</sub> , N <sub>3</sub> Na <sub>4</sub> Re,
<b>11</b>	AgBi <sub>2</sub> ClS <sub>3</sub> , AgBi <sub>2</sub> ClSe <sub>3</sub> , AgBr, AgCl, AgHfRbTe <sub>3</sub> , AgI, Ag <sub>2</sub> Cs <sub>3</sub> S <sub>8</sub> Sb <sub>3</sub> , Ag <sub>2</sub> O <sub>6</sub> Te <sub>2</sub> , Ag <sub>8</sub> BaS <sub>5</sub> , AlAs <sub>3</sub> Cl <sub>4</sub> S <sub>5</sub> , AlAu, AlCl <sub>6</sub> NS <sub>2</sub> , AlCs <sub>6</sub> Sb <sub>3</sub> , AlF <sub>4</sub> K, AlI <sub>4</sub> In, AlRb <sub>6</sub> Sb <sub>3</sub> , Al <sub>2</sub> As <sub>3</sub> K <sub>3</sub> , Al <sub>2</sub> CaO <sub>4</sub> , Al <sub>2</sub> Na <sub>7</sub> Sb <sub>5</sub> , Al <sub>3</sub> F <sub>12</sub> NaRb <sub>2</sub> , AsAuK <sub>2</sub> S <sub>4</sub> , AsCs <sub>2</sub> NaO <sub>4</sub> , AsF <sub>5</sub> N <sub>4</sub> S <sub>4</sub> , AsF <sub>8</sub> Sb, AsO <sub>4</sub> Sb, As <sub>2</sub> Te <sub>3</sub> , As <sub>3</sub> BrO <sub>6</sub> Pb <sub>2</sub> , As <sub>3</sub> Cs <sub>6</sub> In, As <sub>3</sub> F <sub>6</sub> SbSe <sub>4</sub> , As <sub>4</sub> S <sub>5</sub> , AuK <sub>2</sub> PS <sub>4</sub> , AuPS <sub>4</sub> Tl <sub>2</sub> , AuSr, Au <sub>2</sub> BaSb <sub>2</sub> , BBeLi, BBr <sub>3</sub> P <sub>4</sub> S <sub>3</sub> , BS <sub>3</sub> Tl <sub>3</sub> , BSe <sub>3</sub> Tl <sub>3</sub> , BaBi <sub>2</sub> Pd <sub>2</sub> , BaIn <sub>2</sub> P <sub>2</sub> , BaNaO <sub>7</sub> ScSi <sub>2</sub> , BaO <sub>10</sub> Sc <sub>2</sub> Si <sub>3</sub> , BaO <sub>10</sub> Si <sub>3</sub> Y <sub>2</sub> , BaO <sub>3</sub> Se,

Part 2 of all the predicted materials with band crossings from **Cases 1 or 2:**

	BaO <sub>3</sub> Te, BaPd <sub>2</sub> S <sub>4</sub> , BaS <sub>3</sub> Sn <sub>2</sub> , BaSb <sub>2</sub> , Ba <sub>2</sub> BrP <sub>7</sub> , Ba <sub>2</sub> ClF <sub>7</sub> Zn <sub>2</sub> , Ba <sub>2</sub> ClP <sub>7</sub> , Ba <sub>2</sub> GaGeN, Ba <sub>2</sub> GeSe <sub>2</sub> Te <sub>2</sub> , Ba <sub>2</sub> GeSe <sub>4</sub> , Ba <sub>2</sub> IP <sub>7</sub> , Ba <sub>2</sub> LiN <sub>4</sub> Re, Ba <sub>2</sub> Se <sub>4</sub> Si, Ba <sub>2</sub> SiTe <sub>4</sub> , Ba <sub>3</sub> Bi <sub>6</sub> PbSe <sub>13</sub> , Ba <sub>3</sub> Ge <sub>2</sub> N <sub>2</sub> , Ba <sub>4</sub> Cl <sub>2</sub> N <sub>4</sub> W, Ba <sub>4</sub> Ga <sub>2</sub> S <sub>7</sub> , Bi, BiCdClO <sub>2</sub> , Bi <sub>2</sub> Ga <sub>2</sub> In <sub>4</sub> S <sub>12</sub> , Bi <sub>2</sub> In <sub>4</sub> S <sub>9</sub> , Bi <sub>2</sub> Pd <sub>2</sub> Sr, Bi <sub>6</sub> Se <sub>13</sub> Sr <sub>4</sub> , Bi <sub>7</sub> In <sub>3</sub> Pb <sub>4</sub> S <sub>18</sub> , Bi <sub>8</sub> Cs <sub>2</sub> Se <sub>13</sub> , Bi <sub>8</sub> Rb <sub>2</sub> Se <sub>13</sub> , Br <sub>3</sub> GaLi, Br <sub>3</sub> Nb <sub>3</sub> Se <sub>10</sub> , Br <sub>4</sub> K <sub>2</sub> Zn, Br <sub>5</sub> CsHg <sub>2</sub> , Br <sub>9</sub> TaTe, CAgNO, CAg <sub>2</sub> O <sub>3</sub> , CaF <sub>3</sub> K, CaSb <sub>2</sub> , Ca <sub>2</sub> O <sub>12</sub> Si <sub>4</sub> Zr, Ca <sub>5</sub> N <sub>4</sub> O <sub>2</sub> W, Ca <sub>7</sub> N <sub>9</sub> NbSi <sub>2</sub> , CdCs <sub>2</sub> I <sub>4</sub> , Cl <sub>12</sub> Re <sub>2</sub> S, Cl <sub>13</sub> PRE <sub>2</sub> , ClF <sub>5</sub> NRe, ClIn <sub>5</sub> S <sub>5</sub> , ClIn <sub>5</sub> Se <sub>5</sub> , ClKO <sub>3</sub> , Cl <sub>2</sub> O <sub>11</sub> Te <sub>6</sub> , Cl <sub>3</sub> GeRb, Cl <sub>3</sub> N <sub>3</sub> S <sub>3</sub> , Cl <sub>3</sub> Nb <sub>3</sub> Se <sub>10</sub> , Cl <sub>6</sub> Pd <sub>6</sub> S <sub>6</sub> , Cl <sub>7</sub> CsTi <sub>2</sub> , Cl <sub>7</sub> Nb <sub>3</sub> Se <sub>5</sub> , Cs <sub>2</sub> HgI <sub>4</sub> , Cs <sub>3</sub> I <sub>4</sub> Li, Cs <sub>6</sub> GaSb <sub>3</sub> , F <sub>11</sub> In <sub>3</sub> Rb <sub>2</sub> , F <sub>14</sub> Sb <sub>4</sub> , FKO <sub>2</sub> S, FKO <sub>2</sub> Se, FLiO <sub>4</sub> SiSr <sub>2</sub> , FO <sub>3</sub> SeY, F <sub>4</sub> MgSr, F <sub>7</sub> In <sub>2</sub> K, F <sub>7</sub> PbTa, F <sub>7</sub> SrTa, F <sub>8</sub> LiNaY <sub>2</sub> , GaGeNSr <sub>2</sub> , GaGe <sub>2</sub> Na <sub>5</sub> , GaI <sub>3</sub> Li, Ga <sub>5</sub> Pt, GeHfPd, GeS <sub>4</sub> Sr <sub>2</sub> , Ge <sub>2</sub> N <sub>2</sub> Sr <sub>3</sub> , Ge <sub>4</sub> K <sub>4</sub> Se <sub>10</sub> , HfS <sub>3</sub> , HfSe <sub>3</sub> , HfSe <sub>3</sub> Tl <sub>2</sub> , HfTe <sub>3</sub> , I <sub>2</sub> Zr, I <sub>9</sub> Re <sub>3</sub> , InNa <sub>5</sub> S <sub>4</sub> , In <sub>2</sub> S <sub>7</sub> Sn <sub>3</sub> , In <sub>5</sub> S <sub>6</sub> Tl, In <sub>5</sub> Se <sub>7</sub> Tl, In <sub>6</sub> S <sub>7</sub> , In <sub>6</sub> Se <sub>7</sub> , K <sub>2</sub> O <sub>5</sub> S <sub>2</sub> , K <sub>4</sub> P <sub>8</sub> Te <sub>4</sub> , LaS <sub>3</sub> Y, Li <sub>4</sub> ReSr <sub>2</sub> , Li <sub>2</sub> O <sub>7</sub> Ti <sub>3</sub> , Li <sub>4</sub> S <sub>4</sub> Si, MgZn <sub>2</sub> , MoO <sub>3</sub> , MoTe <sub>2</sub> , Mo <sub>2</sub> O <sub>9</sub> Zn <sub>3</sub> , Mo <sub>2</sub> S <sub>3</sub> , N <sub>2</sub> O <sub>4</sub> , NaNb <sub>3</sub> O <sub>16</sub> Te <sub>4</sub> , Na <sub>2</sub> O <sub>7</sub> Ti <sub>3</sub> , Na <sub>2</sub> P <sub>2</sub> S <sub>6</sub> , NbPt <sub>3</sub> , Nb <sub>2</sub> P <sub>2</sub> Rb <sub>2</sub> S <sub>11</sub> , Nb <sub>2</sub> Se <sub>3</sub> , O <sub>2</sub> Te, O <sub>3</sub> P <sub>4</sub> S <sub>6</sub> , O <sub>3</sub> PbS, O <sub>3</sub> PbSe, O <sub>3</sub> PdSe, O <sub>3</sub> SeSr, O <sub>3</sub> Tl <sub>4</sub> , O <sub>6</sub> P <sub>4</sub> , O <sub>6</sub> Pb <sub>3</sub> S, O <sub>7</sub> PbTi <sub>3</sub> , O <sub>7</sub> Si <sub>2</sub> Y <sub>2</sub> , O <sub>9</sub> S <sub>2</sub> Zn <sub>3</sub> , P <sub>4</sub> S <sub>5</sub> , P <sub>4</sub> S <sub>6</sub> , P <sub>5</sub> Y, PbS, Pb <sub>9</sub> Rb <sub>4</sub> , Pt <sub>3</sub> Ta, Pt <sub>6</sub> Si <sub>5</sub> , S <sub>3</sub> Ti, S <sub>3</sub> Tl <sub>2</sub> Zr, S <sub>3</sub> Y <sub>2</sub> , S <sub>4</sub> SiSr <sub>2</sub> , S <sub>7</sub> Sb <sub>4</sub> Sn, Sb, Sb <sub>2</sub> Sr, Se <sub>3</sub> Ta, Se <sub>3</sub> Ta <sub>2</sub> , Se <sub>3</sub> Zr, Sn <sub>2</sub> SrZn <sub>2</sub> , Te <sub>3</sub> Zr,
11	
13	Al <sub>2</sub> Cl <sub>8</sub> Sr, Br <sub>3</sub> NbSe, Br <sub>6</sub> Nb <sub>2</sub> Se <sub>2</sub> , Cl <sub>3</sub> NbSe, FMo <sub>2</sub> O <sub>7</sub> Y, I <sub>4</sub> Zr, I <sub>6</sub> Nb <sub>2</sub> Te <sub>2</sub> ,
14	Ag <sub>2</sub> HgS <sub>2</sub> , Ag <sub>2</sub> O <sub>3</sub> S, Ag <sub>2</sub> Te, AlBr <sub>3</sub> , AlCaF <sub>5</sub> , AlCl <sub>4</sub> Li, AlI <sub>3</sub> , AlNa <sub>3</sub> S <sub>3</sub> , Al <sub>2</sub> B <sub>2</sub> Cs <sub>2</sub> O <sub>7</sub> , Al <sub>2</sub> Br <sub>6</sub> , Al <sub>2</sub> Br <sub>6</sub> N <sub>2</sub> Se <sub>2</sub> , Al <sub>2</sub> Cl <sub>6</sub> OSn, AsBaKSe <sub>3</sub> , AsISe, AsLuSe, AsNaS <sub>2</sub> , AsSY, AsSeY, As <sub>2</sub> F <sub>12</sub> Hg <sub>3</sub> , As <sub>2</sub> F <sub>8</sub> O <sub>2</sub> Rb <sub>2</sub> , As <sub>2</sub> Pt <sub>2</sub> Sr, As <sub>2</sub> S <sub>3</sub> , As <sub>2</sub> Se <sub>3</sub> , AuCl <sub>3</sub> , AuITe, AuI <sub>4</sub> Li, AuNaSe <sub>2</sub> , BN, B <sub>2</sub> Mg <sub>2</sub> O <sub>5</sub> , BaBeLa <sub>2</sub> O <sub>5</sub> , BaGa <sub>2</sub> Pt <sub>2</sub> , BaKSbSe <sub>3</sub> , BaNb <sub>2</sub> O <sub>6</sub> , BaP <sub>2</sub> , BaS <sub>2</sub> Sn, Ba <sub>2</sub> Br <sub>5</sub> Cs, Ba <sub>2</sub> ClCs <sub>4</sub> Sn, Ba <sub>3</sub> P <sub>14</sub> , BeLiN, Bi, BiBr <sub>3</sub> , BrInTe, Br <sub>2</sub> O <sub>5</sub> Sb <sub>4</sub> , Br <sub>3</sub> Ga, Br <sub>6</sub> Hg <sub>3</sub> Se <sub>2</sub> Zr, CF <sub>4</sub> , CKNSe, C <sub>2</sub> Ca, C <sub>2</sub> Cl <sub>4</sub> S <sub>2</sub> , C <sub>7</sub> Y <sub>4</sub> , Cd <sub>2</sub> K <sub>2</sub> O <sub>3</sub> , Cl <sub>2</sub> MgO <sub>8</sub> , Cl <sub>2</sub> OS, Cl <sub>2</sub> O <sub>5</sub> Sb <sub>4</sub> , Cl <sub>2</sub> Te <sub>3</sub> , Cl <sub>4</sub> Hg <sub>4</sub> I <sub>2</sub> S, Cl <sub>4</sub> IK, Cl <sub>6</sub> Hg <sub>3</sub> S <sub>2</sub> Zr, FGaO <sub>3</sub> Te, FMoO <sub>4</sub> Y, FO <sub>3</sub> SeY, F <sub>4</sub> Zr, GaI <sub>3</sub> , HfO <sub>2</sub> , Hg <sub>2</sub> MoO <sub>4</sub> , Hg <sub>2</sub> O <sub>3</sub> Se, IIInTe, ILiO <sub>4</sub> , I <sub>2</sub> Pd, I <sub>2</sub> Pt, I <sub>3</sub> Sb, I <sub>5</sub> Nb, I <sub>6</sub> In <sub>2</sub> , KNaO <sub>2</sub> Zn, KPS <sub>4</sub> Sn, K <sub>2</sub> O <sub>7</sub> W <sub>2</sub> , K <sub>2</sub> Se <sub>3</sub> Te, LaSbSe, LiP, Lu <sub>2</sub> O <sub>5</sub> Si, NOTa, Na <sub>2</sub> O <sub>3</sub> Zn <sub>2</sub> , Na <sub>2</sub> Se <sub>3</sub> Sn, O <sub>2</sub> Ti, O <sub>3</sub> Pb <sub>2</sub> , O <sub>3</sub> S, O <sub>6</sub> Se <sub>2</sub> Ti, O <sub>7</sub> P <sub>2</sub> Sn <sub>2</sub> , O <sub>7</sub> Rb <sub>2</sub> W <sub>2</sub> , O <sub>7</sub> Si <sub>2</sub> Y <sub>2</sub> , Rb <sub>2</sub> S <sub>7</sub> Sb <sub>4</sub> , Rb <sub>2</sub> Te <sub>3</sub> Zr,
15	AllaO <sub>3</sub> , B <sub>4</sub> O <sub>8</sub> U, Ba <sub>2</sub> Re <sub>6</sub> S <sub>11</sub> , Be <sub>2</sub> La <sub>2</sub> O <sub>5</sub> , Br <sub>6</sub> Cs <sub>3</sub> La, Br <sub>6</sub> In <sub>2</sub> Th, C <sub>2</sub> Br <sub>10</sub> La <sub>6</sub> , C <sub>3</sub> K <sub>4</sub> O <sub>11</sub> U, Cl <sub>11</sub> NRe <sub>2</sub> S <sub>2</sub> , ClLa <sub>3</sub> O <sub>8</sub> Si <sub>2</sub> , ClLa <sub>3</sub> S <sub>8</sub> Si <sub>2</sub> , Cl <sub>5</sub> Pa, Cl <sub>6</sub> ReTes, Cs <sub>2</sub> F <sub>7</sub> Pa, Cs <sub>2</sub> Re <sub>3</sub> Se <sub>6</sub> , Cs <sub>4</sub> Re <sub>6</sub> S <sub>13</sub> , Cs <sub>4</sub> Re <sub>6</sub> Se <sub>13</sub> , F <sub>3</sub> La <sub>2</sub> LiO <sub>8</sub> S <sub>2</sub> , F <sub>4</sub> LiLu, F <sub>7</sub> K <sub>2</sub> Pa, F <sub>7</sub> PaRb <sub>2</sub> , GaLa <sub>2</sub> N <sub>3</sub> , ILa <sub>3</sub> S <sub>8</sub> Si <sub>2</sub> , I <sub>4</sub> U, InS <sub>2</sub> Tl, In <sub>2</sub> Na <sub>6</sub> S <sub>6</sub> , In <sub>2</sub> Te <sub>5</sub> , KNaO <sub>3</sub> Ti, KO <sub>2</sub> Sb, KO <sub>8</sub> W <sub>2</sub> Y, KS <sub>2</sub> Sb, K <sub>2</sub> MoO <sub>2</sub> S <sub>2</sub> , K <sub>2</sub> Mo <sub>3</sub> O <sub>10</sub> , K <sub>2</sub> Mo <sub>3</sub> O <sub>12</sub> Th, K <sub>2</sub> O <sub>4</sub> Zn <sub>3</sub> , K <sub>2</sub> O <sub>7</sub> Se <sub>2</sub> , K <sub>2</sub> Rb <sub>2</sub> Re <sub>6</sub> S <sub>13</sub> , K <sub>2</sub> Re <sub>3</sub> S <sub>6</sub> , K <sub>2</sub> Re <sub>3</sub> Se <sub>6</sub> , K <sub>2</sub> S <sub>3</sub> Ti, K <sub>2</sub> S <sub>5</sub> Sn <sub>2</sub> , K <sub>2</sub> S <sub>7</sub> Sb <sub>4</sub> , K <sub>2</sub> Se <sub>5</sub> Sn <sub>2</sub> , K <sub>3</sub> NaO <sub>8</sub> W <sub>2</sub> , K <sub>4</sub> Re <sub>6</sub> Se <sub>12</sub> , K <sub>4</sub> S <sub>14</sub> Ti <sub>3</sub> , K <sub>6</sub> Nb <sub>4</sub> S <sub>22</sub> , K <sub>6</sub> S <sub>22</sub> Ta <sub>4</sub> , K <sub>6</sub> Sb <sub>3</sub> Tl <sub>2</sub> , La <sub>2</sub> O <sub>11</sub> Te <sub>4</sub> , LiMo <sub>2</sub> O <sub>8</sub> Sb, LiO <sub>6</sub> ScSi <sub>2</sub> , Li <sub>2</sub> O <sub>8</sub> Ta <sub>3</sub> , Li <sub>2</sub> S <sub>2</sub> Sn, Li <sub>2</sub> O <sub>3</sub> Pb, Li <sub>2</sub> O <sub>3</sub> Sn, Li <sub>2</sub> O <sub>3</sub> Te, Li <sub>2</sub> O <sub>3</sub> Ti, Li <sub>2</sub> O <sub>3</sub> Zr, Li <sub>2</sub> O <sub>4</sub> W, Li <sub>2</sub> S <sub>3</sub> Sn, Li <sub>3</sub> Na <sub>5</sub> S <sub>8</sub> Ti <sub>2</sub> , Li <sub>3</sub> O <sub>4</sub> Ta, Li <sub>4</sub> O <sub>5</sub> Se, Li <sub>6</sub> O <sub>7</sub> Zr <sub>2</sub> , LuO <sub>4</sub> Ta, MgO, Mg <sub>2</sub> O <sub>8</sub> Te <sub>3</sub> , MoNa <sub>2</sub> O <sub>12</sub> Te <sub>4</sub> , MoO <sub>2</sub> Rb <sub>2</sub> S <sub>2</sub> , MoO <sub>6</sub> Y <sub>2</sub> , MoP <sub>4</sub> , Mo <sub>2</sub> O <sub>8</sub> Zr, Mo <sub>3</sub> Na <sub>2</sub> O <sub>12</sub> Zr, Mo <sub>3</sub> O <sub>10</sub> Rb <sub>2</sub> , Mo <sub>7</sub> O <sub>22</sub> Tl <sub>2</sub> , N <sub>2</sub> OSi <sub>2</sub> , N <sub>2</sub> O <sub>2</sub> S <sub>2</sub> Se, N <sub>2</sub> O <sub>2</sub> S <sub>3</sub> , N <sub>3</sub> NbSr <sub>2</sub> , N <sub>3</sub> Si <sub>2</sub> Ta, N <sub>4</sub> Se <sub>4</sub> , N <sub>6</sub> S <sub>5</sub> , NaNb <sub>2</sub> PS <sub>10</sub> , NaO <sub>2</sub> Y, NaO <sub>3</sub> RbTi, NaO <sub>6</sub> ScSi <sub>2</sub> , NaS <sub>2</sub> Sb,

Part 3 of all the predicted materials with band crossings from **Cases 1 or 2:**

15	NaSi, Na <sub>2</sub> Nb <sub>4</sub> O <sub>11</sub> , Na <sub>2</sub> O <sub>11</sub> Si <sub>4</sub> Zr, Na <sub>2</sub> O <sub>12</sub> Te <sub>4</sub> W, Na <sub>2</sub> O <sub>3</sub> Pt, Na <sub>2</sub> O <sub>6</sub> Si <sub>2</sub> Zn, Na <sub>2</sub> O <sub>7</sub> Sb <sub>4</sub> , Na <sub>2</sub> O <sub>7</sub> Si <sub>3</sub> , Na <sub>2</sub> Re <sub>3</sub> S <sub>6</sub> , Na <sub>2</sub> Re <sub>3</sub> Se <sub>6</sub> , Na <sub>2</sub> Se <sub>3</sub> Te, Na <sub>2</sub> Sn <sub>4</sub> Sr, Na <sub>4</sub> O <sub>10</sub> Te <sub>4</sub> , Na <sub>4</sub> S <sub>8</sub> Sn <sub>3</sub> , Na <sub>4</sub> Si <sub>4</sub> , Na <sub>5</sub> NbO <sub>5</sub> , Na <sub>5</sub> O <sub>5</sub> Ta, Na <sub>6</sub> S <sub>7</sub> Sn <sub>2</sub> , Na <sub>6</sub> Sb <sub>4</sub> Tl, Na <sub>6</sub> Se <sub>2</sub> Si <sub>2</sub> , Na <sub>6</sub> Se <sub>7</sub> Sn <sub>2</sub> , NbO <sub>4</sub> Y, Nb <sub>2</sub> O <sub>5</sub> , Nb <sub>2</sub> O <sub>6</sub> Sn, O <sub>11</sub> Te <sub>4</sub> Y <sub>2</sub> , O <sub>2</sub> RbSb, O <sub>2</sub> Si, O <sub>3</sub> SiZn, O <sub>4</sub> PdS, O <sub>4</sub> PdSe, O <sub>4</sub> Rb <sub>2</sub> Zn <sub>3</sub> , O <sub>4</sub> Sb <sub>2</sub> , O <sub>4</sub> WZn, O <sub>5</sub> Pb <sub>2</sub> Te, O <sub>5</sub> PdSe <sub>2</sub> , O <sub>5</sub> STi, O <sub>5</sub> Sb <sub>2</sub> , O <sub>5</sub> Ta <sub>2</sub> , O <sub>5</sub> Ti <sub>3</sub> , O <sub>6</sub> Pb <sub>2</sub> SbY, O <sub>6</sub> Sn <sub>3</sub> W, O <sub>6</sub> TeZn <sub>3</sub> , O <sub>7</sub> Rb <sub>2</sub> Se <sub>2</sub> , O <sub>7</sub> SnTa <sub>2</sub> , O <sub>8</sub> P <sub>2</sub> Pb <sub>3</sub> , O <sub>8</sub> P <sub>4</sub> , O <sub>8</sub> Te <sub>3</sub> Zn <sub>2</sub> , O <sub>9</sub> Rb <sub>6</sub> Te <sub>2</sub> , O <sub>9</sub> Si <sub>3</sub> Sr <sub>3</sub> , P <sub>2</sub> Pt <sub>5</sub> , P <sub>2</sub> Rb <sub>4</sub> Se <sub>9</sub> , P <sub>2</sub> S <sub>7</sub> Zr, P <sub>4</sub> S <sub>4</sub> , P <sub>6</sub> Pt <sub>4</sub> Sr, Pb <sub>8</sub> Tl <sub>2</sub> Zr, PbSe <sub>4</sub> Tl <sub>2</sub> Zr, Pb <sub>3</sub> S <sub>15</sub> Sb <sub>8</sub> , Pb <sub>5</sub> S <sub>17</sub> Sb <sub>8</sub> , Pb <sub>9</sub> Pd <sub>13</sub> , Rb <sub>2</sub> Re <sub>3</sub> S <sub>6</sub> , Rb <sub>2</sub> Re <sub>3</sub> Se <sub>6</sub> , Rb <sub>2</sub> Se <sub>5</sub> Sn <sub>2</sub> , Rb <sub>4</sub> Re <sub>6</sub> S <sub>12</sub> , Rb <sub>4</sub> Re <sub>6</sub> S <sub>13</sub> , Rb <sub>4</sub> Re <sub>6</sub> Se <sub>12</sub> , Rb <sub>4</sub> S <sub>14</sub> Ti <sub>3</sub> , Rb <sub>4</sub> Se <sub>14</sub> Zr <sub>3</sub> , Rb <sub>4</sub> Te <sub>16</sub> Zr <sub>3</sub> , Re <sub>2</sub> Sc <sub>3</sub> Si <sub>4</sub> , Re <sub>3</sub> S <sub>6</sub> Tl <sub>2</sub> , Re <sub>3</sub> Se <sub>6</sub> Tl <sub>2</sub> , Re <sub>6</sub> Se <sub>12</sub> Tl <sub>4</sub> , S <sub>10</sub> , STa <sub>6</sub> , S <sub>3</sub> Sn <sub>2</sub> Tl <sub>2</sub> , S <sub>5</sub> Sn <sub>2</sub> Tl <sub>2</sub> , Sb <sub>2</sub> Te <sub>3</sub> , Se <sub>3</sub> Tl <sub>2</sub> , Se <sub>4</sub> SiTl <sub>4</sub> , TeTl <sub>2</sub> , Te <sub>3</sub> Tl <sub>2</sub> ,
16	AlPS <sub>4</sub> , C <sub>11</sub> N <sub>4</sub> ,
17	Ag <sub>2</sub> Se, B <sub>18</sub> Cs <sub>2</sub> O <sub>28</sub> , C <sub>2</sub> BN, F <sub>10</sub> In <sub>3</sub> Rb, NaNbO <sub>3</sub> ,
19	AgCsSe <sub>4</sub> , AgHgIS, AgLuSe <sub>2</sub> , AgNO <sub>3</sub> , AgRbSe <sub>4</sub> , AgScSe <sub>2</sub> , AgSe <sub>2</sub> Y, Ag <sub>2</sub> GeO <sub>3</sub> , Ag <sub>2</sub> INO <sub>3</sub> , Ag <sub>2</sub> O <sub>3</sub> Si, Ag <sub>2</sub> O <sub>3</sub> Sn, Ag <sub>2</sub> S, Ag <sub>2</sub> Se, Ag <sub>3</sub> B <sub>5</sub> O <sub>9</sub> , Ag <sub>3</sub> IN <sub>2</sub> O <sub>6</sub> , Ag <sub>4</sub> P <sub>2</sub> S <sub>6</sub> , AlBaF <sub>5</sub> , AlBaLaO <sub>4</sub> , AlCl <sub>4</sub> Na, Al <sub>2</sub> Ca <sub>3</sub> N <sub>4</sub> , Al <sub>2</sub> N <sub>2</sub> O <sub>3</sub> SiSr, AsBr <sub>3</sub> , AsClO <sub>2</sub> Pb, AsCl <sub>3</sub> , AsCl <sub>3</sub> F <sub>6</sub> S, AsK, AsKM <sub>0</sub> O <sub>15</sub> , AsKO <sub>3</sub> , AsKO <sub>9</sub> W <sub>2</sub> , AsNa, AsNaO <sub>9</sub> W <sub>2</sub> , AsO <sub>5</sub> Sb, AsRb, As <sub>2</sub> F <sub>12</sub> Se <sub>4</sub> Te <sub>2</sub> , As <sub>2</sub> Na <sub>4</sub> Te <sub>4</sub> , As <sub>2</sub> O <sub>5</sub> , BGe <sub>2</sub> KO <sub>6</sub> , B <sub>2</sub> BaO <sub>6</sub> Zn <sub>2</sub> , B <sub>2</sub> Ba <sub>3</sub> N <sub>4</sub> , B <sub>2</sub> Ca <sub>2</sub> O <sub>5</sub> , B <sub>2</sub> O <sub>7</sub> Se <sub>2</sub> , B <sub>3</sub> F <sub>3</sub> Li <sub>2</sub> O <sub>4</sub> , B <sub>3</sub> LiO <sub>7</sub> Rb, B <sub>6</sub> Cs <sub>2</sub> O <sub>10</sub> , BaBiSe <sub>3</sub> , BaF <sub>5</sub> Ga, BaGeO <sub>3</sub> , BaGeO <sub>4</sub> Pb, BaN <sub>2</sub> O <sub>4</sub> , BaO <sub>3</sub> Si, BaSbTe <sub>3</sub> , Ba <sub>5</sub> N <sub>6</sub> Si <sub>2</sub> , Ba <sub>6</sub> Se <sub>13</sub> Sn <sub>6</sub> , BeCaFNaO <sub>6</sub> Si <sub>2</sub> , BeF <sub>3</sub> Rb, BiClO <sub>3</sub> Se, BiCl <sub>2</sub> KO <sub>4</sub> S, BiSe <sub>3</sub> Sr, Bi <sub>2</sub> I <sub>4</sub> O <sub>13</sub> , Bi <sub>4</sub> Cl <sub>14</sub> Se <sub>10</sub> , BrNO <sub>3</sub> , Br <sub>3</sub> Sb, Br <sub>4</sub> CsTl, Br <sub>4</sub> InNa, Br <sub>5</sub> PbTl <sub>3</sub> , CO <sub>2</sub> , CO <sub>4</sub> Pb <sub>2</sub> , C <sub>2</sub> F <sub>2</sub> O <sub>3</sub> , C <sub>2</sub> F <sub>5</sub> O <sub>4</sub> RbSb <sub>2</sub> , C <sub>2</sub> N <sub>2</sub> Se <sub>2</sub> , C <sub>4</sub> AlBa <sub>2</sub> LiN <sub>8</sub> , C <sub>4</sub> BF <sub>12</sub> K, C <sub>4</sub> O <sub>4</sub> Tl <sub>2</sub> , CdCs <sub>2</sub> Ge <sub>3</sub> Se <sub>8</sub> , CdCs <sub>2</sub> Se <sub>8</sub> Sn <sub>3</sub> , CdI <sub>2</sub> O <sub>6</sub> , Cd <sub>2</sub> O <sub>12</sub> Rb <sub>2</sub> S <sub>3</sub> , Cl <sub>14</sub> Ga <sub>3</sub> Sb <sub>7</sub> Se <sub>8</sub> , ClF <sub>3</sub> Sn <sub>2</sub> , Cl <sub>2</sub> S, Cl <sub>2</sub> Si, Cl <sub>4</sub> Cs <sub>2</sub> Hg, Cl <sub>4</sub> GaN <sub>a</sub> , Cl <sub>5</sub> N <sub>3</sub> OP <sub>2</sub> S, Cl <sub>5</sub> N <sub>3</sub> S <sub>4</sub> Se, Cs <sub>11</sub> O <sub>3</sub> Rb <sub>7</sub> , CsSb, Cs <sub>2</sub> Ge <sub>3</sub> MgSe <sub>8</sub> , Cs <sub>2</sub> Ge <sub>3</sub> Se <sub>8</sub> Zn, Cs <sub>2</sub> Ge <sub>3</sub> Te <sub>8</sub> Zn, Cs <sub>2</sub> HgS <sub>8</sub> Sn <sub>3</sub> , Cs <sub>2</sub> HgSe <sub>8</sub> Sn <sub>3</sub> , Cs <sub>2</sub> MgSe <sub>8</sub> Sn <sub>3</sub> , Cs <sub>2</sub> S <sub>5</sub> , Cs <sub>2</sub> Se <sub>5</sub> , Cs <sub>2</sub> Se <sub>8</sub> Sn <sub>3</sub> Zn, F <sub>10</sub> IN <sub>3</sub> O <sub>3</sub> , FIO <sub>2</sub> , F <sub>2</sub> Ge, F <sub>2</sub> Sn, F <sub>3</sub> K <sub>2</sub> O <sub>4</sub> SSb, F <sub>4</sub> S, F <sub>4</sub> Se, F <sub>4</sub> Te, F <sub>5</sub> Na <sub>2</sub> Sb, F <sub>6</sub> Na <sub>3</sub> NbO, GeI <sub>3</sub> Rb, GeO <sub>4</sub> PbSr, ISSb, I <sub>5</sub> PbTl <sub>3</sub> , KLi <sub>2</sub> NaO <sub>8</sub> S <sub>2</sub> , KP, KP <sub>2</sub> Se <sub>6</sub> Y, K <sub>2</sub> S <sub>5</sub> , K <sub>2</sub> Se <sub>5</sub> , LaN <sub>5</sub> Si <sub>3</sub> , La <sub>2</sub> O <sub>6</sub> Te, Li <sub>3</sub> P <sub>7</sub> , MoNa <sub>4</sub> O <sub>14</sub> S <sub>3</sub> , NaP, Na <sub>4</sub> SnTe <sub>4</sub> , NbO <sub>5</sub> RbSi, O <sub>2</sub> Rb <sub>2</sub> Sn, O <sub>2</sub> Si, O <sub>2</sub> Te, O <sub>3</sub> Sb <sub>2</sub> , O <sub>3</sub> Xe, O <sub>4</sub> SeTl <sub>2</sub> , O <sub>6</sub> TeY <sub>2</sub> , O <sub>6</sub> WY <sub>2</sub> , PPbRbS <sub>4</sub> , RbSb, Rb <sub>2</sub> S <sub>5</sub> , Rb <sub>2</sub> Se <sub>5</sub> , S <sub>17</sub> Sb <sub>6</sub> Sr <sub>6</sub> , S <sub>5</sub> Tl <sub>2</sub> ,
20	AgAsK <sub>2</sub> , AgAsNa <sub>2</sub> , AgBiK <sub>2</sub> , AgK <sub>2</sub> Sb, AlF <sub>5</sub> Tl <sub>2</sub> , AlO <sub>4</sub> P, AsGaO <sub>4</sub> , B <sub>3</sub> Ba <sub>3</sub> BrO <sub>9</sub> Pb <sub>2</sub> , B <sub>5</sub> Cs <sub>2</sub> Li <sub>3</sub> O <sub>10</sub> , BaNb <sub>2</sub> O <sub>6</sub> , BaO <sub>3</sub> Ti, Ba <sub>6</sub> OS <sub>15</sub> Ti <sub>5</sub> , BeLi <sub>2</sub> O <sub>4</sub> Si, BeO <sub>6</sub> P <sub>2</sub> , Bi <sub>2</sub> K <sub>4</sub> Zn, Br <sub>4</sub> Cs <sub>3</sub> Li, CCaO <sub>3</sub> , CMgO <sub>3</sub> , CdO <sub>10</sub> Pb <sub>6</sub> Te, ClF <sub>5</sub> GeO <sub>2</sub> , FInO <sub>5</sub> Te <sub>2</sub> , F <sub>3</sub> ISn <sub>2</sub> , InNa <sub>2</sub> , K <sub>2</sub> O <sub>6</sub> Si <sub>2</sub> Zn, Na <sub>2</sub> Tl, NbSe <sub>2</sub> , O <sub>13</sub> P <sub>4</sub> Y <sub>2</sub> , O <sub>2</sub> Si, O <sub>7</sub> TaY <sub>3</sub> ,
21	O <sub>8</sub> U <sub>3</sub> ,
25	Ag <sub>3</sub> Sb, AsGa, Bi <sub>4</sub> Br <sub>2</sub> O <sub>9</sub> Te <sub>2</sub> , CB <sub>2</sub> N, C <sub>2</sub> BN, CaMoO <sub>6</sub> Sr <sub>2</sub> , CaO <sub>6</sub> Sr <sub>2</sub> W, Ca <sub>2</sub> O <sub>6</sub> PdW, CdO <sub>6</sub> Sr <sub>2</sub> W, CdTe, HfNO <sub>3</sub> Ta, InSb, SiTi,
26	AgNbO <sub>3</sub> , B <sub>2</sub> K <sub>3</sub> Nb <sub>3</sub> O <sub>12</sub> , BaCdK <sub>2</sub> SB <sub>2</sub> , BaHgS <sub>2</sub> , Br <sub>4</sub> CsLi <sub>3</sub> , CaF <sub>2</sub> , CaNO <sub>2</sub> Ta, CaPPt, CdK <sub>2</sub> SB <sub>2</sub> Sr, CdO <sub>3</sub> Ti, Cl <sub>2</sub> O <sub>2</sub> W, F <sub>13</sub> RbTh <sub>3</sub> , F <sub>13</sub> Th <sub>3</sub> Tl, Ge <sub>3</sub> NaP <sub>3</sub> , In <sub>11</sub> Mo <sub>40</sub> O <sub>62</sub> , KPSe <sub>6</sub> Zr, MoPt <sub>2</sub> Si <sub>3</sub> , NaNbO <sub>3</sub> , Na <sub>2</sub> O <sub>5</sub> SiTi, O <sub>2</sub> Se, O <sub>3</sub> Pb <sub>2</sub> , P <sub>5</sub> Tl,

Part 4 of all the predicted materials with band crossings from **Cases 1 or 2:**

26	Pb <sub>3</sub> S <sub>12</sub> Sn <sub>3</sub> Y <sub>2</sub> ,
29	AgIO <sub>3</sub> , BNa <sub>5</sub> O <sub>16</sub> S <sub>4</sub> , B <sub>3</sub> BiO <sub>6</sub> , B <sub>7</sub> ClMg <sub>3</sub> O <sub>13</sub> , Ba <sub>2</sub> N <sub>5</sub> O <sub>10</sub> Tl, BiIO <sub>4</sub> , Bi <sub>2</sub> FNbO <sub>5</sub> , Bi <sub>2</sub> MoO <sub>6</sub> , C <sub>2</sub> Cl <sub>2</sub> Hg <sub>3</sub> N <sub>4</sub> , C <sub>2</sub> FNOS, CaO <sub>3</sub> Te, CdI <sub>2</sub> O <sub>6</sub> , CdN <sub>2</sub> O <sub>6</sub> , Cl <sub>11</sub> Mo <sub>3</sub> N <sub>2</sub> , ClFO <sub>2</sub> S, Cs <sub>4</sub> GeP <sub>4</sub> Se <sub>12</sub> , Cs <sub>4</sub> S <sub>11</sub> Ta <sub>2</sub> , F <sub>16</sub> PdXe <sub>2</sub> , F <sub>2</sub> IKO <sub>2</sub> , F <sub>2</sub> OSe, F <sub>4</sub> RbTl, F <sub>4</sub> SW, GaLaOSe <sub>2</sub> , GeKNO, GeP <sub>4</sub> Rb <sub>4</sub> Se <sub>12</sub> , GePtS, GePtSe, Ge <sub>4</sub> LiNaO <sub>9</sub> , Ge <sub>4</sub> Li <sub>2</sub> O <sub>9</sub> , Ge <sub>4</sub> Se <sub>9</sub> , HgN <sub>6</sub> , InNb <sub>8</sub> Te <sub>2</sub> , KPSe <sub>6</sub> , K <sub>2</sub> MgO <sub>4</sub> Si, K <sub>2</sub> O <sub>4</sub> SiZn, K <sub>4</sub> Nb <sub>2</sub> S <sub>11</sub> , LiNOSi, Mg <sub>2</sub> O <sub>6</sub> Si <sub>2</sub> , NaNbO <sub>3</sub> , O <sub>2</sub> Zr, O <sub>5</sub> TeU, P <sub>6</sub> Rb <sub>4</sub> Se <sub>12</sub> ,
31	AgCd <sub>2</sub> GaS <sub>4</sub> , Ag <sub>2</sub> CdGeS <sub>4</sub> , Ag <sub>2</sub> HgSe <sub>4</sub> Sn, Ag <sub>2</sub> I <sub>4</sub> Zn, Ag <sub>3</sub> AsS <sub>4</sub> , Ag <sub>3</sub> PS <sub>4</sub> , Ag <sub>3</sub> PSe <sub>4</sub> , Al <sub>4</sub> BaS <sub>7</sub> , As <sub>4</sub> K <sub>7</sub> Nb, As <sub>4</sub> NbRb <sub>7</sub> , BBaClF <sub>4</sub> , B <sub>3</sub> Be <sub>2</sub> KO <sub>7</sub> , B <sub>3</sub> Be <sub>2</sub> O <sub>7</sub> Rb, B <sub>4</sub> CaO <sub>7</sub> , B <sub>4</sub> HgO <sub>7</sub> , B <sub>4</sub> O <sub>7</sub> Sn, BaBe <sub>2</sub> O <sub>7</sub> Si <sub>2</sub> , BaGa <sub>4</sub> S <sub>7</sub> , Ba <sub>2</sub> N <sub>8</sub> Si <sub>5</sub> , BrIn <sub>5</sub> S <sub>5</sub> , BrIn <sub>5</sub> Se <sub>5</sub> , CGaNSi, CLi <sub>4</sub> O <sub>4</sub> , C <sub>6</sub> Cs <sub>3</sub> N <sub>6</sub> NaRe <sub>6</sub> Se <sub>8</sub> , CaCl <sub>2</sub> , CdGeLi <sub>2</sub> O <sub>4</sub> , CdGeLi <sub>2</sub> S <sub>4</sub> , CdLi <sub>2</sub> S <sub>4</sub> Sn, CdO <sub>4</sub> S, Cd <sub>3</sub> Na <sub>6</sub> O <sub>18</sub> Si <sub>6</sub> , Ge <sub>16</sub> K <sub>14</sub> Zn, Ge <sub>16</sub> Rb <sub>14</sub> Zn, HfN <sub>3</sub> Ta, HgO <sub>4</sub> S, I <sub>2</sub> Zr, I <sub>4</sub> Te, K <sub>10</sub> MgMo <sub>7</sub> O <sub>27</sub> , MoNNa <sub>3</sub> O <sub>3</sub> , N <sub>8</sub> Si <sub>5</sub> Sr <sub>2</sub> , NaNbO <sub>3</sub> , OSn, O <sub>7</sub> STe <sub>2</sub> , S <sub>3</sub> Sb <sub>2</sub> , Te <sub>2</sub> W,
33	AgAsS, AlF <sub>6</sub> Li <sub>3</sub> , AlGeLi <sub>3</sub> O <sub>5</sub> , AlLiO <sub>4</sub> Si, AlO <sub>4</sub> RbSi, AlO <sub>4</sub> SiTl, Al <sub>2</sub> Rb <sub>4</sub> S <sub>5</sub> , AsBeCsO <sub>4</sub> , AsK <sub>3</sub> S <sub>4</sub> , AsLiMoO <sub>6</sub> , AsLi <sub>3</sub> S <sub>3</sub> , AuSbTl, Ba <sub>2</sub> Ge <sub>2</sub> Te <sub>5</sub> , BeF <sub>4</sub> Na <sub>2</sub> , BeN <sub>2</sub> Si, BiCl <sub>3</sub> , Bi <sub>2</sub> O <sub>7</sub> Ti <sub>2</sub> , BrNZn <sub>2</sub> , C <sub>15</sub> N <sub>3</sub> O <sub>12</sub> Re <sub>3</sub> , CBr <sub>2</sub> Se <sub>4</sub> , C <sub>4</sub> N <sub>4</sub> PbS <sub>4</sub> Zn, CaF <sub>22</sub> P <sub>2</sub> Xe <sub>5</sub> , CaGa <sub>2</sub> O <sub>4</sub> , Ca <sub>2</sub> Nb <sub>2</sub> O <sub>7</sub> , CdNaO <sub>4</sub> P, CdP <sub>2</sub> , Cl <sub>10</sub> Re <sub>6</sub> Te <sub>8</sub> , ClF <sub>11</sub> Sb <sub>2</sub> Xe, Cl <sub>4</sub> GaHg <sub>2</sub> Sb, Cl <sub>4</sub> Rb <sub>2</sub> Zn, Cl <sub>7</sub> Ga <sub>2</sub> In, Cl <sub>7</sub> Ga <sub>2</sub> K, Cl <sub>7</sub> Ga <sub>3</sub> , CsIMoO <sub>6</sub> , CsO <sub>7</sub> SbSi <sub>2</sub> , F <sub>2</sub> O <sub>4</sub> RbSSb, F <sub>5</sub> KNaNbO, F <sub>5</sub> K <sub>2</sub> Y, F <sub>6</sub> KNaSn, F <sub>6</sub> N <sub>3</sub> P <sub>3</sub> , GaGeLi <sub>3</sub> O <sub>5</sub> , GaLiS <sub>2</sub> , GaLiSe <sub>2</sub> , GaNaO <sub>2</sub> , GeKNaO <sub>3</sub> , GeKO <sub>5</sub> P, GeO <sub>5</sub> RbSb, Ge <sub>2</sub> Na <sub>2</sub> Se <sub>5</sub> , Hg <sub>2</sub> O <sub>5</sub> Te, Hg <sub>5</sub> I <sub>6</sub> Sb <sub>2</sub> , ILiO <sub>3</sub> , INaO <sub>3</sub> , ISSb, InLiS <sub>2</sub> , InLiSe <sub>2</sub> , KLiO <sub>4</sub> S, KO <sub>5</sub> SbSi, LaLu <sub>3</sub> , LaO <sub>3</sub> Y, LaS <sub>2</sub> , La <sub>2</sub> O <sub>7</sub> Ti <sub>2</sub> , LiP <sub>5</sub> , Li <sub>2</sub> S, MgN <sub>2</sub> Si, MgNa <sub>2</sub> O <sub>4</sub> Si, Mg <sub>2</sub> O <sub>6</sub> Si <sub>2</sub> , Mo <sub>3</sub> O <sub>16</sub> Tl <sub>2</sub> U <sub>2</sub> , N <sub>2</sub> SiZn, NaNbO <sub>3</sub> , NaO <sub>3</sub> Ta, NaO <sub>4</sub> SiY, NaO <sub>6</sub> Se <sub>2</sub> Y, Na <sub>2</sub> O <sub>3</sub> S <sub>2</sub> , Na <sub>4</sub> O <sub>13</sub> Sc <sub>2</sub> Si <sub>4</sub> , NbO <sub>4</sub> Sb, O <sub>2</sub> Sb, O <sub>2</sub> Si, O <sub>4</sub> SbTa, O <sub>4</sub> Sb <sub>2</sub> , PS <sub>4</sub> SnTl, P <sub>4</sub> Se <sub>5</sub> , S <sub>3</sub> ScY, S <sub>3</sub> Sc <sub>2</sub> , S <sub>3</sub> Sr <sub>2</sub> Zn,
36	Ag <sub>10</sub> Br <sub>3</sub> Te <sub>4</sub> , AgS <sub>3</sub> Ta, Ag <sub>2</sub> GeS <sub>3</sub> , Ag <sub>2</sub> HgI <sub>2</sub> S, Ag <sub>5</sub> S <sub>4</sub> Sb, AlBaN <sub>5</sub> O <sub>3</sub> Si <sub>4</sub> , Al <sub>2</sub> BaN <sub>4</sub> O <sub>4</sub> Si <sub>3</sub> , Al <sub>6</sub> Ca <sub>5</sub> O <sub>14</sub> , AsBiCa <sub>2</sub> O <sub>6</sub> , AsBiCd <sub>2</sub> O <sub>6</sub> , AsCs <sub>2</sub> LiO <sub>4</sub> , AsLiO <sub>4</sub> Rb <sub>2</sub> , As <sub>2</sub> Ca <sub>2</sub> Cd, As <sub>2</sub> Cl <sub>13</sub> Sb, Au <sub>2</sub> Ga, Au <sub>2</sub> O <sub>10</sub> Se <sub>3</sub> , B <sub>2</sub> O <sub>3</sub> , BaBi <sub>2</sub> Nb <sub>2</sub> O <sub>9</sub> , BaF <sub>4</sub> Mg, BaF <sub>4</sub> Zn, BaMo <sub>2</sub> O <sub>11</sub> Se <sub>2</sub> , BaO <sub>4</sub> W, BaO <sub>7</sub> Si <sub>2</sub> Zn <sub>2</sub> , BaP <sub>10</sub> , Ba <sub>2</sub> BiInS <sub>5</sub> , Ba <sub>2</sub> GaTe <sub>5</sub> Y, Ba <sub>2</sub> InSbSe <sub>5</sub> , Ba <sub>2</sub> InSe <sub>5</sub> Y, Ba <sub>2</sub> InTe <sub>5</sub> Y, Ba <sub>4</sub> Sb <sub>2</sub> Se <sub>11</sub> Si, BiPbPd <sub>2</sub> , BiPd, Bi <sub>2</sub> CaO <sub>9</sub> Ta <sub>2</sub> , Bi <sub>2</sub> GeO <sub>5</sub> , Bi <sub>2</sub> Nb <sub>2</sub> O <sub>9</sub> Pb, Bi <sub>2</sub> O <sub>5</sub> Si, Bi <sub>2</sub> O <sub>9</sub> SrTa <sub>2</sub> , BrCl, BrF <sub>5</sub> , BrI, C, CAI <sub>4</sub> O <sub>4</sub> , CClF <sub>3</sub> , CLi <sub>4</sub> O <sub>4</sub> , C <sub>3</sub> Al <sub>7</sub> N <sub>3</sub> , Ca <sub>3</sub> O <sub>7</sub> Ti <sub>2</sub> , ClIn, ClN <sub>3</sub> , CsI <sub>2</sub> Li, Cs <sub>2</sub> F <sub>3</sub> Li, Cs <sub>2</sub> I <sub>3</sub> Li, Cs <sub>2</sub> O <sub>3</sub> Pb, Cs <sub>2</sub> S <sub>2</sub> Te, Cs <sub>2</sub> S <sub>3</sub> , Cs <sub>2</sub> S <sub>3</sub> Ti, Cs <sub>2</sub> Se <sub>3</sub> , Cs <sub>2</sub> Te <sub>3</sub> , F <sub>2</sub> NP, F <sub>3</sub> K <sub>3</sub> O <sub>4</sub> Ti, F <sub>4</sub> MgSr, GaInS <sub>3</sub> , GaO <sub>6</sub> Y <sub>3</sub> , GaS <sub>6</sub> Y <sub>3</sub> , Ga <sub>2</sub> GeLa <sub>2</sub> S <sub>8</sub> , GeLi <sub>2</sub> O <sub>3</sub> , GeNa <sub>2</sub> O <sub>3</sub> , GeTe <sub>4</sub> Zr, Ge <sub>2</sub> LiN <sub>3</sub> , Ge <sub>2</sub> N <sub>2</sub> O, Ge <sub>2</sub> N <sub>3</sub> Na, Ge <sub>6</sub> La <sub>4</sub> Mg <sub>5</sub> , Ge <sub>6</sub> Lu <sub>4</sub> Zn <sub>5</sub> , Ge <sub>6</sub> Y <sub>4</sub> Zn <sub>5</sub> , Hg <sub>2</sub> O <sub>3</sub> Se, I <sub>2</sub> O <sub>7</sub> Ti, I <sub>4</sub> Nb, In <sub>2</sub> Na <sub>5</sub> Te <sub>6</sub> , K <sub>2</sub> O <sub>3</sub> Pb, K <sub>2</sub> S <sub>3</sub> , K <sub>2</sub> Se <sub>3</sub> , K <sub>3</sub> S <sub>4</sub> Sb, LaO <sub>4</sub> Ta, LiN <sub>3</sub> Si <sub>2</sub> , Li <sub>2</sub> NO <sub>2</sub> P, Li <sub>2</sub> O <sub>3</sub> Si, Li <sub>2</sub> O <sub>8</sub> Sn <sub>3</sub> Zn, Mg <sub>2</sub> N <sub>3</sub> P, Mg <sub>2</sub> O <sub>4</sub> Si, MoP <sub>2</sub> , NN <sub>5</sub> O <sub>4</sub> W, N <sub>2</sub> OSi <sub>2</sub> , N <sub>3</sub> NaSi <sub>2</sub> , N <sub>3</sub> PZn <sub>2</sub> , Na <sub>2</sub> O <sub>3</sub> Si, Na <sub>2</sub> O <sub>7</sub> W <sub>2</sub> , Na <sub>2</sub> PdS <sub>2</sub> , Na <sub>2</sub> PdSe <sub>2</sub> , Na <sub>2</sub> PtS <sub>2</sub> , Na <sub>2</sub> PtSe <sub>2</sub> , NbS <sub>2</sub> , Nb <sub>2</sub> O <sub>7</sub> Sr <sub>2</sub> , OSn, O <sub>3</sub> PbRb <sub>2</sub> , O <sub>5</sub> Pb <sub>3</sub> Se, O <sub>7</sub> Sr <sub>2</sub> Ta <sub>2</sub> , PSi, P <sub>2</sub> W, PbS, Pd <sub>2</sub> Sb, Rb <sub>2</sub> S <sub>3</sub> , Rb <sub>2</sub> Se <sub>3</sub> , Sc <sub>9</sub> Te <sub>2</sub> ,
38	La <sub>4</sub> O <sub>4</sub> Se <sub>3</sub> , O <sub>8</sub> U <sub>3</sub> , Re <sub>2</sub> ScSi <sub>3</sub> , Re <sub>5</sub> Sc <sub>5</sub> Si <sub>12</sub> ,
40	Br <sub>3</sub> Cl <sub>9</sub> Cs <sub>3</sub> Re <sub>3</sub> , Cl <sub>12</sub> Cs <sub>3</sub> Re <sub>3</sub> , Cl <sub>4</sub> CsRe,

Part 5 of all the predicted materials with band crossings from **Cases 1 or 2**:

43	<chem>AgN2NaO4</chem> , <chem>Ag2O3</chem> , <chem>AlNaP2S6</chem> , <chem>Al22Mo5</chem> , <chem>As3PbS6Tl</chem> , <chem>As4Sr3</chem> , <chem>Au2O3</chem> , <chem>BaBr2O6</chem> , <chem>BaCdSe4Sn</chem> , <chem>BaCl2O6</chem> , <chem>BaF6Te</chem> , <chem>Ba3P4</chem> , <chem>CCl2F2</chem> , <chem>Ca2GePd2</chem> , <chem>Cd7P10</chem> , <chem>Cl12HfSe2</chem> , <chem>Cl12MoSe2</chem> , <chem>Cl12Se2Zr</chem> , <chem>Cl2O2S</chem> , <chem>Cl2O6Pb</chem> , <chem>Cl2O6Sr</chem> , <chem>Cl2S2</chem> , <chem>Cs2Se</chem> , <chem>F4Pd</chem> , <chem>F4Pt</chem> , <chem>Ga2GeLi2S6</chem> , <chem>Ga2GeS6Sn</chem> , <chem>GeS2</chem> , <chem>GeSe2</chem> , <chem>HfP2S6</chem> , <chem>I4S16Sn</chem> , <chem>InSr</chem> , <chem>N6O14Zn</chem> , <chem>Na2O6Si2Zn</chem> , <chem>O2Si</chem> , <chem>O5P2</chem> , <chem>P2S6Ti</chem> , <chem>P4Sr3</chem> , <chem>PdS4U2</chem> ,
44	<chem>AgNO2</chem> , <chem>Ag8S</chem> , <chem>AlF7MgNa2</chem> , <chem>Al2As2Cs2O7</chem> , <chem>AsGa</chem> , <chem>AuCaSn</chem> , <chem>AuGeNa</chem> , <chem>BBeLi</chem> , <chem>BN</chem> , <chem>BaCaGa4O8</chem> , <chem>BaN8OSi6</chem> , <chem>BaN8Si6</chem> , <chem>Ba3Se7Th</chem> , <chem>Ba5In4S7Te4</chem> , <chem>CO5U</chem> , <chem>Cl5Cs2Li3</chem> , <chem>GeLuPd</chem> , <chem>GePdY</chem> , <chem>GePtU</chem> , <chem>HgO</chem> , <chem>NNaO2</chem> , <chem>N5P3</chem> , <chem>N8Si6Sr</chem> , <chem>NaPd3Si2</chem> ,
46	<chem>AlF7MgNa2</chem> , <chem>Ba2GaInO5</chem> , <chem>Ba2In2O5</chem> , <chem>Ca2Ga2O5</chem> , <chem>Cd2Nb2O7</chem> , <chem>Cl9PSe</chem> , <chem>GaO5ScSr2</chem> , <chem>In2O5Sr2</chem> , <chem>NbReSi</chem> , <chem>ReSiTa</chem> ,
48	<chem>O2Si</chem> ,
49	<chem>O5Ta2</chem> ,
50	<chem>C</chem> , <chem>O2Si</chem> ,
51	<chem>AgBrHgS</chem> , <chem>AgHgIS</chem> , <chem>AlPt2</chem> , <chem>As2Br2Cd2Hg2</chem> , <chem>AuCsTe</chem> , <chem>AuITe2</chem> , <chem>AuRbTe</chem> , <chem>Au3Rb2Tl</chem> , <chem>BLi</chem> , <chem>BaNb2O6</chem> , <chem>BiPd3</chem> , <chem>Br11CsNb4</chem> , <chem>Br11Nb4Rb</chem> , <chem>Br6SrTh</chem> , <chem>CB2U</chem> , <chem>C3AlY3</chem> , <chem>C3I6OY7</chem> , <chem>Ca5P6Pd6</chem> , <chem>CdMg</chem> , <chem>Cl11CsNb4</chem> , <chem>Cl11Nb4Rb</chem> , <chem>Cl19LiNb6</chem> , <chem>Cl2Mg</chem> , <chem>GaPt2</chem> , <chem>K2S</chem> , <chem>La2Se9U2</chem> , <chem>MoPt</chem> , <chem>O5U2</chem> , <chem>PdTi</chem> , <chem>PtTi</chem> ,
52	<chem>Ag4Bi2O5</chem> , <chem>Ag6BaO4</chem> , <chem>Ag6O4Sr</chem> , <chem>Al2Ba3N4</chem> , <chem>Al2N4Sr3</chem> , <chem>AsGeSe</chem> , <chem>As4Ga3K3</chem> , <chem>BaCl4Zn</chem> , <chem>Ba3Ga2N4</chem> , <chem>Ba3GeMgN4</chem> , <chem>BiNbO4</chem> , <chem>BiO4Ta</chem> , <chem>Bi3BrO4</chem> , <chem>Br4Ga2</chem> , <chem>Br4InK</chem> , <chem>Br4In2</chem> , <chem>Br4KTL</chem> , <chem>Br4Tl2</chem> , <chem>Ca2GeIn2Sr</chem> , <chem>Cl4Ga2</chem> , <chem>FO3ScTe</chem> , <chem>F7HfKPd</chem> , <chem>F7KPdZr</chem> , <chem>Ga2N4Sr3</chem> , <chem>GeMgN4Sr3</chem> , <chem>Hf2K2O5</chem> , <chem>I4In2</chem> , <chem>K2O5Zr2</chem> , <chem>LiO3Sb</chem> , <chem>NbO4Sb</chem> , <chem>O4SnW</chem> ,
53	<chem>AgISe3</chem> , <chem>AgITe3</chem> , <chem>F7KSnZr</chem> ,
54	<chem>AgClO2</chem> , <chem>Au2Cd2Rb2S4</chem> , <chem>BiGaO3</chem> , <chem>ClF8Nb</chem> , <chem>ClF8Ta</chem> , <chem>O2Si</chem> ,
55	<chem>AgAsHg2O4</chem> , <chem>AgK5N2O6</chem> , <chem>AlGeO5Y</chem> , <chem>Al2Bi6Ca5</chem> , <chem>Al2Ca5Sb6</chem> , <chem>Al4Bi2O9</chem> , <chem>Al5NaO12Ti2</chem> , <chem>AsKS5Sn</chem> , <chem>As2F16MgXe2</chem> , <chem>As2Ge</chem> , <chem>As2O6Zn3</chem> , <chem>As2Si</chem> , <chem>As3Ca4</chem> , <chem>As3Sr4</chem> , <chem>As6Ca5Ga2</chem> , <chem>As6Ca5Sn2</chem> , <chem>As6Sn2Sr5</chem> , <chem>AuI2K5O2</chem> , <chem>Au3O2Rb5</chem> , <chem>BTa4Te8</chem> , <chem>B4MoU</chem> , <chem>B4MoY</chem> , <chem>B4UW</chem> , <chem>B4WY</chem> , <chem>B6ReSc2</chem> , <chem>B6ReY2</chem> , <chem>B6U2W</chem> , <chem>BaNb8O14</chem> , <chem>Ba3OSb2</chem> , <chem>Ba5In2Sb6</chem> , <chem>Bi2Ga4O9</chem> , <chem>Bi6In2Sr5</chem> , <chem>Bi8Ca3Pd4</chem> , <chem>Br5Nb</chem> , <chem>CB2Lu</chem> , <chem>C2B2Sc</chem> , <chem>C5Y4</chem> , <chem>CaGe2O5</chem> , <chem>Ca2O4Pb</chem> , <chem>Ca3O6Tl2</chem> , <chem>Ca5Ga2Sb6</chem> , <chem>Ca5In2Sb6</chem> , <chem>CdCl4Na2</chem> , <chem>CdO4U</chem> , <chem>Cd2I7Tl3</chem> , <chem>Cd2O4Sn</chem> , <chem>Cd7Th6</chem> , <chem>Cl4MgNa2</chem> , <chem>Cl4Na2Ti</chem> , <chem>Cs2Te2</chem> , <chem>Ga2Mg</chem> , <chem>Ga5NaO12Ti2</chem> , <chem>HfO3Pb</chem> , <chem>HfReSi2</chem> , <chem>I6PbTl4</chem> , <chem>InLa2Si2</chem> , <chem>In2Sb6Sr5</chem> , <chem>In3NaS5</chem> , <chem>La2S5Sn</chem> , <chem>Li7Si2</chem> , <chem>Mg2O4Si</chem> , <chem>Na2O4U</chem> , <chem>Nb2Pd3Se8</chem> , <chem>Nb4SiTe4</chem> , <chem>Nb8O14Sr</chem> , <chem>O2Se</chem> , <chem>O3PbZr</chem> , <chem>O4Pb2Pt</chem> , <chem>O4Pb3</chem> , <chem>O6Sr3Tl2</chem> , <chem>O8W3</chem> , <chem>P6Sn2Sr5</chem> , <chem>Pb4S11Sb4</chem> , <chem>PdSe2Tl2</chem> , <chem>Pd3Se8Ta2</chem> , <chem>Pt3S8Ta2</chem> , <chem>Pt3Sc2Si2</chem> , <chem>Pt3Se8Ta2</chem> , <chem>Pt7Sc4Si2</chem> , <chem>Pt7Zn12</chem> , <chem>Rb2Te2</chem> , <chem>ReSi2Zr</chem> , <chem>Se2Ti9</chem> , <chem>Se9Sn2Sr4</chem> , <chem>SiTa4Te4</chem> ,
56	<chem>BiLiO3</chem> , <chem>Bi2O3</chem> , <chem>Cl6Se4Zr</chem> , <chem>I11Nb6</chem> , <chem>Li2O5Te2</chem> , <chem>Na2O4U</chem> , <chem>O2Si</chem> , <chem>O3Sb2</chem> , <chem>O4SnSr2</chem> ,
57	<chem>AgNbO3</chem> , <chem>AlLu</chem> , <chem>AsCa2ClO4</chem> , <chem>AsKO2</chem> , <chem>AsNa5O5</chem> , <chem>AsO2Rb</chem> , <chem>As2Cl3Hg3Tl</chem> , <chem>AuCs2PS4</chem> , <chem>AuLaO3</chem> , <chem>AuRb2S4Sb</chem> , <chem>BaF4OTi</chem> , <chem>BaF5Sb</chem> , <chem>Bi3F6N</chem> , <chem>Br3Hg3Sb2Tl</chem> , <chem>Br5P</chem> , <chem>CaNb2O4</chem> , <chem>Ca3Ga2Pd2</chem> , <chem>Ca3Ga2Pt2</chem> , <chem>Cl6HfTe6</chem> , <chem>Cl6Te6Zr</chem> , <chem>Cl7Re3Se7</chem> , <chem>CsP7</chem> , <chem>Cs2Te13</chem> , <chem>F5KTe</chem> , <chem>F5SbSr</chem> , <chem>F9SbSn3</chem> , <chem>GaLaOS2</chem> , <chem>HgK2S2</chem> , <chem>La2O2S2</chem> , <chem>Li2O7Si3</chem> , <chem>N5NbSr5</chem> , <chem>NaNbO3</chem> , <chem>NaO4TiY</chem> ,

Part 6 of all the predicted materials with band crossings from **Cases 1 or 2:**

57	<b>OPb, O<sub>5</sub>TeU, STa<sub>2</sub>,</b>
58	Ag <sub>5</sub> O <sub>4</sub> Si, Al <sub>2</sub> O <sub>5</sub> Si, <b>AsTa<sub>2</sub>, As<sub>2</sub>Ti, As<sub>4</sub>Ca<sub>3</sub>In<sub>2</sub>, AuKNa<sub>2</sub>O<sub>2</sub>, AuNa<sub>2</sub>O<sub>2</sub>Rb, Au<sub>8</sub>Sn<sub>3</sub>Sr<sub>3</sub>, B, B<sub>28</sub>, B<sub>2</sub>CaLi<sub>4</sub>O<sub>6</sub>, B<sub>2</sub>Cd<sub>3</sub>O<sub>6</sub>, B<sub>2</sub>Mg<sub>3</sub>O<sub>6</sub>, Bi<sub>2</sub>Hf, Bi<sub>2</sub>O<sub>2</sub>S, Bi<sub>2</sub>Zr, Bi<sub>3</sub>RbS<sub>5</sub>, Br<sub>16</sub>Ti<sub>7</sub>, Br<sub>2</sub>Ca, CO<sub>2</sub>, C<sub>2</sub>B<sub>2</sub>Mg, C<sub>3</sub>Al<sub>2</sub>Th<sub>2</sub>, C<sub>3</sub>Mg<sub>2</sub>, CaCl<sub>2</sub>, Ca<sub>2</sub>Ge<sub>3</sub>Li, Ca<sub>2</sub>LiSi<sub>3</sub>, Cl<sub>16</sub>Ti<sub>7</sub>, ClGaTe, Cl<sub>2</sub>Pd, Cl<sub>2</sub>Pt, Cl<sub>5</sub>NaSn<sub>2</sub>, Cl<sub>5</sub>Nb<sub>3</sub>O<sub>2</sub>, F<sub>12</sub>GeS<sub>2</sub>, F<sub>2</sub>Mg, F<sub>4</sub>Mg<sub>10</sub>O<sub>14</sub>Si<sub>3</sub>, GaLi<sub>3</sub>Na<sub>2</sub>O<sub>4</sub>, GeO<sub>2</sub>, Ge<sub>6</sub>Li<sub>2</sub>Sr<sub>4</sub>, HfSb<sub>2</sub>, I<sub>2</sub>Li<sub>5</sub>S<sub>3</sub>Sb, I<sub>2</sub>Pd, InK<sub>2</sub>Na<sub>3</sub>O<sub>4</sub>, InNa<sub>3</sub>O<sub>4</sub>Rb<sub>2</sub>, InS, In<sub>2</sub>P<sub>4</sub>Sr<sub>3</sub>, In<sub>2</sub>Se, In<sub>2</sub>Te, In<sub>4</sub>Se<sub>3</sub>, In<sub>4</sub>Te<sub>3</sub>, K<sub>2</sub>Na<sub>3</sub>O<sub>4</sub>Tl, La<sub>2</sub>Mo<sub>2</sub>O<sub>7</sub>, La<sub>3</sub>LuSe<sub>6</sub>, Li<sub>3</sub>N<sub>4</sub>NbSr<sub>2</sub>, Li<sub>3</sub>N<sub>4</sub>Sr<sub>2</sub>Ta, N<sub>2</sub>Pd, N<sub>2</sub>Pt, O<sub>2</sub>Pt, O<sub>2</sub>Sn, P<sub>9</sub>Zr<sub>14</sub>, S<sub>12</sub>, STi<sub>2</sub>, SZr<sub>2</sub>, S<sub>2</sub>Ti, Sb<sub>2</sub>Zr, SeTi<sub>2</sub>, SeZr<sub>2</sub>,</b>
59	Ag <sub>3</sub> Sb, AlClO, AlF <sub>4</sub> Rb, AlLi <sub>5</sub> O <sub>4</sub> , AsCl <sub>5</sub> , AsKLi <sub>2</sub> , AsLiMo <sub>2</sub> O <sub>9</sub> , As <sub>5</sub> K <sub>6</sub> Sn <sub>3</sub> , AuCs <sub>3</sub> Ge <sub>4</sub> , AuCs <sub>3</sub> Pb <sub>4</sub> , AuCs <sub>3</sub> Sn <sub>4</sub> , AuGe <sub>4</sub> K <sub>3</sub> , AuGe <sub>4</sub> Rb <sub>3</sub> , AuK <sub>3</sub> Sn <sub>4</sub> , AuPb <sub>4</sub> Rb <sub>3</sub> , AuRb <sub>3</sub> Sn <sub>4</sub> , Au <sub>21</sub> K <sub>12</sub> Sn <sub>4</sub> , Au <sub>3</sub> In, Au <sub>3</sub> In <sub>3</sub> Sr, Au <sub>3</sub> KS <sub>3</sub> , Au <sub>3</sub> Lu, Au <sub>4</sub> S <sub>3</sub> Tl <sub>2</sub> , BCsNa <sub>2</sub> O <sub>3</sub> , BKNa <sub>2</sub> O <sub>3</sub> , BNa <sub>2</sub> O <sub>3</sub> Rb, BaLi <sub>2</sub> Si, BaO <sub>9</sub> Ti <sub>4</sub> , Ba <sub>5</sub> In <sub>4</sub> Sb <sub>6</sub> , Ba <sub>6</sub> Ge <sub>5</sub> N <sub>2</sub> , BrHfN, BrInO, BrLuS, BrNTi, BrNZr, BrOSc, Br <sub>3</sub> Mo, CAgNO, CBiCaFO <sub>4</sub> , CBrN, CCaO <sub>3</sub> , CCIN, CO <sub>5</sub> U, C <sub>2</sub> B <sub>2</sub> Be, CdS, ClInO, ClNTi, Cl <sub>7</sub> Mo <sub>2</sub> O <sub>2</sub> Tl, CsIn <sub>7</sub> S <sub>9</sub> , FNTi, F <sub>3</sub> La, F <sub>4</sub> KSb, GeNa <sub>2</sub> O <sub>5</sub> Ti, Ge <sub>5</sub> N <sub>2</sub> Sr <sub>6</sub> , Hg <sub>3</sub> Pd <sub>8</sub> Se <sub>9</sub> , INTi, INZr, I <sub>3</sub> Ti, I <sub>3</sub> Zr, InNa <sub>5</sub> O <sub>4</sub> , InSb, Li <sub>5</sub> N <sub>4</sub> Re, NaNbO <sub>3</sub> , NaNb <sub>3</sub> O <sub>8</sub> , Pb <sub>2</sub> Pd <sub>3</sub> Te <sub>2</sub> , PdSiY,
60	Ag <sub>3</sub> S <sub>2</sub> Tl, AlCl <sub>4</sub> Hg <sub>2</sub> Sb, AlO <sub>4</sub> Ta, Al <sub>2</sub> Ca <sub>2</sub> O <sub>9</sub> Sn <sub>2</sub> , Al <sub>2</sub> O <sub>3</sub> , As <sub>11</sub> K <sub>3</sub> , As <sub>11</sub> Rb <sub>3</sub> , AsKO <sub>3</sub> , Au <sub>2</sub> F <sub>12</sub> Hg, Au <sub>2</sub> Pb, BaCl <sub>4</sub> Pd, BaCl <sub>4</sub> Zn, BaN <sub>2</sub> O <sub>2</sub> Si <sub>2</sub> , Ba <sub>8</sub> Si <sub>6</sub> Sn, Bi <sub>2</sub> CdGeO <sub>6</sub> , Bi <sub>2</sub> O <sub>3</sub> , BrHg <sub>2</sub> P <sub>3</sub> , CW <sub>2</sub> , CaCl <sub>2</sub> , CaNb <sub>2</sub> O <sub>6</sub> , CaO <sub>4</sub> Te, Ca <sub>3</sub> N <sub>2</sub> , CdK <sub>2</sub> O <sub>2</sub> , CdO <sub>2</sub> Rb <sub>2</sub> , Cl <sub>3</sub> CsLi <sub>2</sub> , Cl <sub>4</sub> LuNa, Cl <sub>4</sub> NaSc, F <sub>2</sub> Zn, F <sub>4</sub> InLi, F <sub>4</sub> Na <sub>2</sub> O <sub>2</sub> W, F <sub>6</sub> NaRbSn, GeO <sub>2</sub> , Hg <sub>3</sub> Rb <sub>2</sub> Te <sub>4</sub> , I <sub>2</sub> O <sub>6</sub> Pb, In <sub>2</sub> O <sub>3</sub> , KM <sub>0</sub> <sub>2</sub> O <sub>8</sub> Y, K <sub>3</sub> P <sub>11</sub> , LiO <sub>6</sub> SbW, Li <sub>2</sub> O <sub>5</sub> Si <sub>2</sub> , MgNb <sub>2</sub> O <sub>6</sub> , MgO <sub>3</sub> Si, MgO <sub>5</sub> Te <sub>2</sub> , Mg <sub>2</sub> O <sub>6</sub> Si <sub>2</sub> , N <sub>4</sub> S <sub>4</sub> , Na <sub>2</sub> O <sub>2</sub> Pb, Na <sub>2</sub> O <sub>4</sub> Te, Na <sub>2</sub> O <sub>5</sub> Si <sub>2</sub> , Na <sub>2</sub> O <sub>9</sub> Si <sub>2</sub> Ti <sub>2</sub> , Na <sub>2</sub> Te <sub>2</sub> , Na <sub>3</sub> P <sub>11</sub> , Nb <sub>2</sub> O <sub>6</sub> Zn, O <sub>2</sub> Pb, O <sub>2</sub> Sn, O <sub>2</sub> Ti, O <sub>3</sub> W, O <sub>4</sub> SrTe, O <sub>5</sub> Se <sub>2</sub> Zn, O <sub>6</sub> Ta <sub>2</sub> Zn, P <sub>11</sub> Rb <sub>3</sub> , PPdS, PPdSe, S <sub>5</sub> Th <sub>2</sub> , Se <sub>5</sub> Th <sub>2</sub> ,
61	AgI <sub>0</sub> <sub>3</sub> , Al <sub>2</sub> Cl <sub>8</sub> Te <sub>4</sub> , AsCd, AsCsSe <sub>2</sub> , AsNaO <sub>2</sub> , AsNaSe <sub>2</sub> , AsS <sub>3</sub> Tl <sub>3</sub> , AsZn, As <sub>3</sub> LaSi, AuSn <sub>2</sub> , Au <sub>3</sub> Ca <sub>7</sub> , B <sub>2</sub> Cl <sub>4</sub> , Ba <sub>2</sub> In <sub>2</sub> Se <sub>5</sub> , Ba <sub>2</sub> Nb <sub>2</sub> O <sub>10</sub> Te, Bi <sub>2</sub> MoO <sub>6</sub> , Bi <sub>2</sub> Pt, Br <sub>5</sub> PdTl <sub>3</sub> , Br <sub>8</sub> Cs <sub>2</sub> Re <sub>2</sub> , C <sub>2</sub> N <sub>2</sub> , C <sub>2</sub> N <sub>2</sub> S, CaN <sub>2</sub> Si, Ca <sub>4</sub> O <sub>10</sub> Ti <sub>3</sub> , CdSb, ClF <sub>3</sub> KSb, ClO <sub>2</sub> , Cl <sub>2</sub> PdSe <sub>8</sub> , Cl <sub>4</sub> Hg <sub>3</sub> Te, FOSb, GaNaO <sub>2</sub> , Ga <sub>2</sub> O <sub>5</sub> Sr <sub>2</sub> , GeLaSe <sub>4</sub> Tl, HfO <sub>2</sub> , HfRb <sub>2</sub> S <sub>4</sub> , HgNa <sub>2</sub> S <sub>2</sub> , HgO <sub>2</sub> , Hg <sub>3</sub> Na <sub>2</sub> S <sub>4</sub> , I <sub>2</sub> O <sub>6</sub> Pd, I <sub>2</sub> Sr, I <sub>4</sub> Pt, K <sub>2</sub> S <sub>4</sub> Zr, LaO <sub>4</sub> Ta, Lu <sub>2</sub> O <sub>4</sub> Pd, Na <sub>2</sub> O <sub>4</sub> U, O <sub>2</sub> Sn, O <sub>2</sub> Te, O <sub>2</sub> Ti, O <sub>2</sub> U, O <sub>3</sub> SeZn, O <sub>3</sub> TeZn, P <sub>4</sub> Re, PdS <sub>2</sub> , PdSe <sub>2</sub> , PtSbSi, PtSiTe, Re <sub>2</sub> Te <sub>5</sub> , Re <sub>6</sub> Se <sub>8</sub> Te <sub>7</sub> , Re <sub>6</sub> Te <sub>15</sub> , S <sub>9</sub> Sb <sub>2</sub> Sn <sub>5</sub> , SbZn,
62	AgBr <sub>3</sub> Cs <sub>2</sub> , AgBr <sub>3</sub> Rb <sub>2</sub> , AgCaSb, AgClO <sub>4</sub> , AgCl <sub>3</sub> Cs <sub>2</sub> , AgCl <sub>3</sub> Rb <sub>2</sub> , AgCs <sub>2</sub> I <sub>3</sub> , AgI <sub>3</sub> K <sub>2</sub> , AgI <sub>3</sub> Rb <sub>2</sub> , AgSTl, AgSeTl, AgTe, AgTeTl, Ag <sub>2</sub> BaTe <sub>2</sub> , Ag <sub>2</sub> CsI <sub>3</sub> , Ag <sub>3</sub> AsSe <sub>3</sub> , AlAs <sub>3</sub> Ca <sub>3</sub> , AlAuCa, AlBMgO <sub>4</sub> , AlBr <sub>4</sub> Cs, AlCa <sub>2</sub> F <sub>7</sub> , AlCa <sub>3</sub> Sb <sub>3</sub> , AlCdF <sub>6</sub> Na, AlCl <sub>4</sub> Cs, AlCl <sub>4</sub> In, AlCl <sub>4</sub> Tl, AlCsF <sub>6</sub> Pd, AlF <sub>4</sub> K, AlF <sub>6</sub> PdRb, AlI <sub>4</sub> Na, AlKSb <sub>4</sub> , AlLaPt, AlLuPt, AlO <sub>3</sub> Sc, AlO <sub>3</sub> Y, AlP <sub>3</sub> Si, AlPdY, AlPtY, Al <sub>2</sub> As <sub>4</sub> Ba <sub>3</sub> , Al <sub>2</sub> BaGe <sub>2</sub> , Al <sub>2</sub> BaSi <sub>2</sub> , Al <sub>2</sub> Ba <sub>3</sub> P <sub>4</sub> , Al <sub>2</sub> BeO <sub>4</sub> , Al <sub>2</sub> CaO <sub>4</sub> , Al <sub>2</sub> Ca <sub>3</sub> Ge <sub>3</sub> , Al <sub>2</sub> F <sub>2</sub> GeO <sub>4</sub> , Al <sub>2</sub> F <sub>2</sub> O <sub>4</sub> Si, Al <sub>2</sub> MgO <sub>4</sub> , Al <sub>2</sub> O <sub>5</sub> Si, Al <sub>2</sub> Sb <sub>6</sub> Sr <sub>5</sub> , Al <sub>3</sub> ITe <sub>3</sub> , AsBaKO <sub>4</sub> , AsBa <sub>2</sub> GaSe <sub>5</sub> , AsCaLi, AsCaNaO <sub>4</sub> ,

Part 7 of all the predicted materials with band crossings from **Cases 1 or 2**:

62	<p>AsCaPd, AsCa<sub>3</sub>N, AsCdNa, AsCd<sub>3</sub>Cl<sub>3</sub>, AsCs<sub>3</sub>Se<sub>4</sub>, AsKMoO<sub>6</sub>, AsK<sub>3</sub>Se<sub>4</sub>, AsLaTe, AsLiMgO<sub>4</sub>, AsLiO<sub>5</sub>Ti, AsLiSr, AsRb<sub>3</sub>Se<sub>4</sub>, AsS<sub>4</sub>Tl<sub>3</sub>, AsSe<sub>4</sub>Tl<sub>3</sub>, As<sub>2</sub>BaZn<sub>2</sub>, As<sub>2</sub>CsSe<sub>3</sub>, As<sub>2</sub>Hf, As<sub>2</sub>Hf<sub>3</sub>, As<sub>2</sub>K<sub>4</sub>Te<sub>4</sub>, As<sub>2</sub>O<sub>4</sub>, As<sub>2</sub>Th, As<sub>2</sub>Zr, As<sub>3</sub>Ba<sub>3</sub>In, As<sub>3</sub>Ca<sub>3</sub>Ga, As<sub>3</sub>ClO<sub>6</sub>Pb<sub>2</sub>, As<sub>3</sub>Cs<sub>5</sub>Ge, As<sub>3</sub>GeKNa<sub>4</sub>, As<sub>3</sub>Hf<sub>5</sub>, As<sub>3</sub>K<sub>5</sub>Pb<sub>3</sub>, As<sub>3</sub>LaZn<sub>3</sub>, As<sub>3</sub>Nb<sub>5</sub>, As<sub>3</sub>OSr<sub>3</sub>Ta, As<sub>3</sub>Rb<sub>5</sub>Si, As<sub>3</sub>Sc<sub>5</sub>, As<sub>4</sub>Cd<sub>2</sub>Ge, As<sub>4</sub>K<sub>6</sub>NbTl, As<sub>4</sub>S<sub>3</sub>, As<sub>4</sub>Se<sub>3</sub>, As<sub>5</sub>Ba<sub>2</sub>In<sub>5</sub>, AuLa, BaLa<sub>2</sub>O<sub>4</sub>, BaLu<sub>2</sub>O<sub>4</sub>, BaLu<sub>2</sub>S<sub>4</sub>, BaLu<sub>2</sub>Te<sub>4</sub>, BaO<sub>3</sub>Th, BaS<sub>3</sub>U, BaSe<sub>5</sub>U<sub>2</sub>, Ba<sub>2</sub>Pb, Ba<sub>2</sub>S<sub>3</sub>Zn, Ba<sub>2</sub>S<sub>4</sub>Ti, Ba<sub>2</sub>Sb<sub>6</sub>Sn<sub>3</sub>, Ba<sub>2</sub>Si, Ba<sub>2</sub>Si<sub>4</sub>, Ba<sub>2</sub>Sn, Ba<sub>2</sub>SnTe<sub>5</sub>, Ba<sub>3</sub>BrGaS<sub>4</sub>, Ba<sub>3</sub>ClGaS<sub>4</sub>, Ba<sub>3</sub>ClGaSe<sub>4</sub>, Ba<sub>3</sub>GaSb<sub>3</sub>, Ba<sub>3</sub>GeO, Ba<sub>3</sub>GeS<sub>5</sub>, Ba<sub>3</sub>S<sub>5</sub>Si, Ba<sub>5</sub>P<sub>4</sub>, Ba<sub>5</sub>Sb<sub>4</sub>, Ba<sub>7</sub>Ge<sub>6</sub>, BeCl<sub>4</sub>Cs<sub>2</sub>, BeCs<sub>2</sub>F<sub>4</sub>, BeF<sub>4</sub>K<sub>2</sub>, BeF<sub>4</sub>Na<sub>2</sub>, BeF<sub>4</sub>Tl<sub>2</sub>, BeO<sub>4</sub>Y<sub>2</sub>, BiBrCdSe<sub>2</sub>, BiBrS, BiBrSe, BiBr<sub>6</sub>Rb<sub>3</sub>, BiCaLi, BiCdClS<sub>2</sub>, BiClS, BiClSe, BiCl<sub>3</sub>O<sub>3</sub>Sr<sub>3</sub>, BiF<sub>3</sub>, BiF<sub>5</sub>K<sub>2</sub>, BiIn<sub>2</sub>Se<sub>4</sub>, BiS, BiSe, BiI<sub>3</sub>, BiInO<sub>3</sub>, BiLiSr, BiMg<sub>2</sub>O<sub>6</sub>P, BiO<sub>6</sub>PPb<sub>2</sub>, Bi<sub>2</sub>CdCs<sub>2</sub>S<sub>5</sub>, Bi<sub>2</sub>Cs<sub>2</sub>S<sub>5</sub>Zn, Bi<sub>2</sub>Cs<sub>2</sub>Se<sub>5</sub>Zn, Bi<sub>2</sub>Ga<sub>4</sub>O<sub>9</sub>, Bi<sub>2</sub>GeO<sub>5</sub>, Bi<sub>2</sub>O<sub>5</sub>Sr<sub>2</sub>, Bi<sub>2</sub>PbS<sub>4</sub>, Bi<sub>2</sub>Pb<sub>2</sub>S<sub>5</sub>, Bi<sub>2</sub>S<sub>3</sub>, Bi<sub>2</sub>S<sub>5</sub>Tl<sub>4</sub>, Bi<sub>2</sub>Se<sub>3</sub>, Bi<sub>3</sub>CsS<sub>5</sub>, Bi<sub>3</sub>CsSe<sub>5</sub>, Bi<sub>3</sub>IIn<sub>2</sub>Se<sub>7</sub>, Bi<sub>3</sub>Sc<sub>5</sub>, Bi<sub>3</sub>Y<sub>5</sub>, Bi<sub>6</sub>Cl<sub>3</sub>FO<sub>7</sub>, BrClPb, BrCsI<sub>2</sub>, BrIPb, BrKO<sub>4</sub>, BrLa<sub>2</sub>S<sub>5</sub>Sb, BrLa<sub>3</sub>Te<sub>4</sub>, BrO<sub>4</sub>Tl, BrSSb, BrTe<sub>2</sub>, Br<sub>2</sub>O<sub>2</sub>Pb<sub>3</sub>, Br<sub>2</sub>Pb, Br<sub>2</sub>S<sub>7</sub>Te, Br<sub>2</sub>Sn, Br<sub>2</sub>Sr, Br<sub>3</sub>CdIn, Br<sub>3</sub>CdRb, Br<sub>3</sub>CdTl, Br<sub>3</sub>Cs, Br<sub>3</sub>CsPb, Br<sub>3</sub>InMg, Br<sub>3</sub>P, Br<sub>3</sub>Sb, Br<sub>4</sub>CdCs<sub>2</sub>, Br<sub>4</sub>CsGa, Br<sub>4</sub>Cs<sub>2</sub>Zn, Br<sub>4</sub>GaN<sub>4</sub>, Br<sub>4</sub>Rb<sub>2</sub>Zn, Br<sub>5</sub>Cs<sub>3</sub>Hg, Br<sub>5</sub>Nb, Br<sub>5</sub>Rb<sub>3</sub>Zn, Br<sub>7</sub>P, C, CLiN, CO<sub>3</sub>Pb, C<sub>2</sub>Ba, C<sub>3</sub>O<sub>2</sub>, Ca, CaCdPd, CaCdPt, CaCd<sub>2</sub>Pd, CaCl<sub>2</sub>, CaF<sub>2</sub>, CaF<sub>3</sub>K, CaGa<sub>2</sub>O<sub>4</sub>, CaGeMg, CaGeMgO<sub>4</sub>, CaGeO<sub>3</sub>, CaGePt, CaGeSr, CaHfS<sub>3</sub>, CaLiN, CaLiSb, CaMgO<sub>4</sub>Si, CaMgPd, CaMgSi, CaMgSn, CaMoO<sub>3</sub>, CaO<sub>3</sub>Pb, CaO<sub>3</sub>Si, CaO<sub>3</sub>Sn, CaO<sub>3</sub>Ti, CaO<sub>3</sub>Zr, CaO<sub>4</sub>S, CaO<sub>4</sub>Sc<sub>2</sub>, CaO<sub>6</sub>Ta<sub>2</sub>, CaPbPd, CaPbPt, CaPbSr, CaPdSn, CaPtSi, CaPtSn, CaS<sub>3</sub>Zr, CaS<sub>4</sub>Sc<sub>2</sub>, CaS<sub>4</sub>Y<sub>2</sub>, CaSe<sub>5</sub>U<sub>2</sub>, CaSiSr, CaSnSr, CaTe, Ca<sub>2</sub>CdSb<sub>2</sub>, Ca<sub>2</sub>Cd<sub>2</sub>KSb<sub>3</sub>, Ca<sub>2</sub>Ge, Ca<sub>2</sub>GeS<sub>4</sub>, Ca<sub>2</sub>Ge<sub>2</sub>InLi, Ca<sub>2</sub>Hg, Ca<sub>2</sub>O<sub>4</sub>Si, Ca<sub>2</sub>Pb, Ca<sub>2</sub>Pt<sub>3</sub>Sn<sub>5</sub>, Ca<sub>2</sub>S<sub>4</sub>Si, Ca<sub>2</sub>S<sub>4</sub>Sn, Ca<sub>2</sub>Se<sub>4</sub>Si, Ca<sub>2</sub>Si, Ca<sub>3</sub>GeO, Ca<sub>3</sub>Hg, Ca<sub>3</sub>InP<sub>3</sub>, Ca<sub>3</sub>OSi, Ca<sub>3</sub>Pd, Ca<sub>6</sub>Cd<sub>11</sub>Pt, Ca<sub>7</sub>Ge<sub>6</sub>, CdClS<sub>2</sub>Sb, CdCl<sub>3</sub>K, CdCl<sub>3</sub>Rb, CdCl<sub>3</sub>Tl, CdCs<sub>2</sub>I<sub>4</sub>, CdCs<sub>3</sub>I<sub>5</sub>, CdF<sub>2</sub>, CdF<sub>3</sub>K, CdGeO<sub>3</sub>, CdGeSr, CdI<sub>3</sub>Tl, CdLi<sub>2</sub>O<sub>4</sub>Si, CdNaSb, CdO<sub>3</sub>Se, CdO<sub>3</sub>Sn, CdO<sub>3</sub>Ti, CdP<sub>14</sub>Pb, CdP<sub>14</sub>Sn, CdPtSr, CdSbTl, Cd<sub>2</sub>GeO<sub>4</sub>, Cd<sub>2</sub>KSb<sub>3</sub>Sr<sub>2</sub>, Cd<sub>3</sub>K<sub>2</sub>S<sub>4</sub>, Cd<sub>3</sub>K<sub>2</sub>Se<sub>4</sub>, Cd<sub>3</sub>K<sub>2</sub>Te<sub>4</sub>, Cd<sub>3</sub>Na<sub>4</sub>Se<sub>5</sub>, Cd<sub>3</sub>Rb<sub>2</sub>S<sub>4</sub>, Cd<sub>3</sub>Rb<sub>2</sub>Se<sub>4</sub>, ClCsO<sub>4</sub>, ClCs<sub>3</sub>O, ClFSn, ClF<sub>3</sub>, ClIPb, ClKO<sub>3</sub>, ClKO<sub>4</sub>, ClK<sub>3</sub>O, ClLaNb<sub>2</sub>O<sub>6</sub>, ClLaSe, ClLaTe, ClLiO<sub>4</sub>, ClLuO<sub>3</sub>Se, ClN<sub>5</sub>S<sub>4</sub>, ClNaO<sub>4</sub>, ClNb<sub>3</sub>O<sub>7</sub>, ClO<sub>3</sub>SbTe, ClO<sub>4</sub>Rb, Cl<sub>2</sub>Hg, Cl<sub>2</sub>O<sub>2</sub>Pb<sub>3</sub>, Cl<sub>2</sub>O<sub>2</sub>U, Cl<sub>2</sub>O<sub>3</sub>Sb<sub>2</sub>Zn, Cl<sub>2</sub>Pb, Cl<sub>2</sub>S<sub>5</sub>Sb<sub>4</sub>, Cl<sub>2</sub>S<sub>7</sub>Te, Cl<sub>2</sub>Sn, Cl<sub>3</sub>GaLi, Cl<sub>3</sub>HgNa, Cl<sub>3</sub>HgTl, Cl<sub>3</sub>KMg, Cl<sub>3</sub>Na, Cl<sub>3</sub>P, Cl<sub>3</sub>Sb, Cl<sub>4</sub>CsGa, Cl<sub>4</sub>Cs<sub>2</sub>Hg, Cl<sub>4</sub>Cs<sub>2</sub>Mg, Cl<sub>4</sub>Cs<sub>2</sub>Zn, Cl<sub>4</sub>GaRb, Cl<sub>4</sub>GaTl, Cl<sub>4</sub>HgK<sub>2</sub>, Cl<sub>4</sub>K<sub>2</sub>Zn, Cl<sub>4</sub>Li<sub>2</sub>Zn, Cl<sub>4</sub>Rb<sub>2</sub>Zn, Cl<sub>5</sub>CsPd<sub>2</sub>, Cl<sub>5</sub>Cs<sub>2</sub>Tl, Cl<sub>5</sub>Cs<sub>3</sub>Hg, Cl<sub>5</sub>K<sub>2</sub>La, Cl<sub>5</sub>Mo, Cl<sub>5</sub>PbRb<sub>3</sub>, Cl<sub>7</sub>InY<sub>2</sub>, CsF<sub>5</sub>Te, CsI, CsIO<sub>4</sub>, CsI<sub>3</sub>, CsI<sub>3</sub>Pb, CsI<sub>3</sub>Sn, CsIn<sub>3</sub>O<sub>5</sub>, CsO<sub>6</sub>ScSe<sub>2</sub>, CsPPbS<sub>4</sub>, CsPPbSe<sub>4</sub>, Cs<sub>2</sub>GaSb<sub>2</sub>, Cs<sub>2</sub>GeTe<sub>4</sub>, Cs<sub>2</sub>MoS<sub>4</sub>, Cs<sub>2</sub>MoSe<sub>4</sub>, Cs<sub>2</sub>O<sub>3</sub>Sn<sub>2</sub>, Cs<sub>2</sub>O<sub>4</sub>Se, Cs<sub>2</sub>O<sub>4</sub>Te, Cs<sub>2</sub>O<sub>4</sub>W, Cs<sub>2</sub>S, Cs<sub>2</sub>S<sub>4</sub>W, Cs<sub>2</sub>Se, Cs<sub>2</sub>Se<sub>4</sub>W, Cs<sub>2</sub>SnTe<sub>4</sub>, Cs<sub>2</sub>Te, Cs<sub>3</sub>I<sub>5</sub>Zn, Cs<sub>3</sub>NbSe<sub>4</sub>, Cs<sub>3</sub>O<sub>4</sub>Sb, Cs<sub>3</sub>PSe<sub>4</sub>, Cs<sub>3</sub>S<sub>4</sub>Sb, Cs<sub>3</sub>S<sub>4</sub>Ta, Cs<sub>3</sub>SbSe<sub>4</sub>, Cs<sub>3</sub>Se<sub>4</sub>Ta, Cs<sub>4</sub>Sb<sub>2</sub>, Cs<sub>5</sub>GeP<sub>3</sub>, Cs<sub>5</sub>P<sub>3</sub>Si, F<sub>10</sub>GeXe, F<sub>11</sub>PtXe, F<sub>11</sub>SbXe, FLa<sub>3</sub>N<sub>4</sub>Si, FLiO<sub>4</sub>SZn, FMoNa<sub>3</sub>O<sub>4</sub>, FNa<sub>3</sub>O<sub>4</sub>W, FOSb, FO<sub>3</sub>STI, FO<sub>4</sub>SY, FSeY, F<sub>2</sub>Ge, F<sub>2</sub>Hg, F<sub>2</sub>Mg, F<sub>2</sub>Mg<sub>3</sub>O<sub>4</sub>Si, F<sub>2</sub>O, F<sub>2</sub>Pb, F<sub>2</sub>S<sub>3</sub>SnSr<sub>2</sub>, F<sub>2</sub>Se<sub>3</sub>SnSr<sub>2</sub>, F<sub>2</sub>Sr, F<sub>3</sub>I,</p>
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Part 8 of all the predicted materials with band crossings from **Cases 1 or 2**:

62	<p><chem>F3MgNa</chem>, <chem>F3NaZn</chem>, <chem>F3PbRb</chem>, <chem>F3Tl</chem>, <chem>F3Y</chem>, <chem>F4GaK</chem>, <chem>F4KTi</chem>, <chem>F4LaRb</chem>, <chem>F5KPd2</chem>, <chem>F5Lu3O2</chem>, <chem>F5NaTe</chem>, <chem>F5RbS</chem>, <chem>F5RbTe</chem>, <chem>F5TeTl</chem>, <chem>F6KNaSi</chem>, <chem>F6Mo</chem>, <chem>F6Pt</chem>, <chem>F6Te</chem>, <chem>F6W</chem>, <chem>F7InMgNa2</chem>, <chem>F7K2Ta</chem>, <chem>F7LiSb2</chem>, <chem>F7NbOSe</chem>, <chem>F8Li4Zr</chem>, <chem>F8Pb2Zr</chem>, <chem>F9KU2</chem>, <chem>GaKO6Se2</chem>, <chem>GaKSb4</chem>, <chem>GaK2Sb2</chem>, <chem>GaLaO3</chem>, <chem>GaLaPd</chem>, <chem>GaLaPd2</chem>, <chem>GaLaPt</chem>, <chem>GaLa3OS5</chem>, <chem>GaLuPd</chem>, <chem>GaLuPt</chem>, <chem>GaNaO6Se2</chem>, <chem>GaPdSc</chem>, <chem>GaPdY</chem>, <chem>GaPd2Y</chem>, <chem>GaPtSc</chem>, <chem>GaPtY</chem>, <chem>GaRb2Sb2</chem>, <chem>GaTh</chem>, <chem>Ga2K2Na4O6</chem>, <chem>Ga2MoO10Te2</chem>, <chem>Ga2Pd5</chem>, <chem>Ga3ITe3</chem>, <chem>Ga3Na2Sb3</chem>, <chem>Ga5Lu3</chem>, <chem>Ga5Y3</chem>, <chem>GeHfMo</chem>, <chem>GeHfPt</chem>, <chem>GeI3Tl</chem>, <chem>GeInLiO4</chem>, <chem>GeLiNbO5</chem>, <chem>GeLiO4Sc</chem>, <chem>GeLi4S4</chem>, <chem>GeLuNaO4</chem>, <chem>GeMgSr</chem>, <chem>GeMg2O4</chem>, <chem>GeMg2S4</chem>, <chem>GeMg2Se4</chem>, <chem>GeMoZr</chem>, <chem>GeNaO4Y</chem>, <chem>GeNa4Se4</chem>, <chem>GeOSr3</chem>, <chem>GeP3Rb5</chem>, <chem>GePd</chem>, <chem>GePdTl</chem>, <chem>GePdU</chem>, <chem>GePdZr</chem>, <chem>GePt</chem>, <chem>GePtU</chem>, <chem>GePtZr</chem>, <chem>GeS</chem>, <chem>GeS3Ti</chem>, <chem>GeSe</chem>, <chem>GeSr2</chem>, <chem>GeTe</chem>, <chem>GeTe3Tl2</chem>, <chem>GeZr</chem>, <chem>Ge2InLiSr2</chem>, <chem>Ge2Li3Na</chem>, <chem>Ge2Mo</chem>, <chem>Ge2Pt3</chem>, <chem>Ge2Sr</chem>, <chem>Ge2W</chem>, <chem>Ge3N4</chem>, <chem>Ge3Pt2</chem>, <chem>Ge4Hf3Nb2</chem>, <chem>Ge4Hf5</chem>, <chem>Ge4Mo3Sc2</chem>, <chem>Ge4Ti5</chem>, <chem>Ge6Sr7</chem>, <chem>HfLa2S5</chem>, <chem>HfLa2Se5</chem>, <chem>HfMoSi</chem>, <chem>HfNbP</chem>, <chem>HfO2</chem>, <chem>HfO3Sr</chem>, <chem>HfP2</chem>, <chem>HfPbS3</chem>, <chem>HfPdSi</chem>, <chem>HfPtSi</chem>, <chem>HfS3Sn</chem>, <chem>HfS3Sr</chem>, <chem>HfS5Y2</chem>, <chem>HfSi</chem>, <chem>HfSiW</chem>, <chem>Hf3P2</chem>, <chem>HgMg2</chem>, <chem>HgO</chem>, <chem>HgO3Se</chem>, <chem>HgP14Sn</chem>, <chem>HgSr3</chem>, <chem>Hg3Sr</chem>, <chem>Hg8Sr</chem>, <chem>IIn3Te3</chem>, <chem>INZn2</chem>, <chem>INaO3</chem>, <chem>INbO2</chem>, <chem>ISSb</chem>, <chem>ISbSe</chem>, <chem>ITe2</chem>, <chem>I2O2Pb3</chem>, <chem>I2P4S3</chem>, <chem>I2P4Se3</chem>, <chem>I2Sr</chem>, <chem>I3PbRb</chem>, <chem>I3Rb</chem>, <chem>I3RbSn</chem>, <chem>I3Tl</chem>, <chem>I4Li2Zn</chem>, <chem>I5Ta</chem>, <chem>I6PdRb2</chem>, <chem>InKO6Te2</chem>, <chem>InLaO3</chem>, <chem>InLiO4Si</chem>, <chem>InP3Sr3</chem>, <chem>InS3Sb</chem>, <chem>InS4SiTl</chem>, <chem>In2KNa9O8</chem>, <chem>In2O3</chem>, <chem>In2O4Sr</chem>, <chem>In2O5Ti</chem>, <chem>In2PbS4</chem>, <chem>In4La2Pd3</chem>, <chem>In5Y3</chem>, <chem>K</chem>, <chem>KNO3</chem>, <chem>KNaS</chem>, <chem>KNaSe</chem>, <chem>KNaTe</chem>, <chem>KO6Se2Y</chem>, <chem>KO6Te2Y</chem>, <chem>KPPbS4</chem>, <chem>KRbS</chem>, <chem>K2MoS4</chem>, <chem>K2Na3P3Si</chem>, <chem>K2O10UW2</chem>, <chem>K2O3Pb</chem>, <chem>K2O3Sn</chem>, <chem>K2O3Zr</chem>, <chem>K2O4S</chem>, <chem>K2O4Se</chem>, <chem>K2P2PdS6</chem>, <chem>K2Se4W</chem>, <chem>K2Te3</chem>, <chem>K3LiSi4</chem>, <chem>K3Li3O6Te</chem>, <chem>K3NO4</chem>, <chem>K3NbS4</chem>, <chem>K3NbSe4</chem>, <chem>K3PS4</chem>, <chem>K3PSe4</chem>, <chem>K3S4Ta</chem>, <chem>K4Se2SnTe2</chem>, <chem>K4Se4Sn</chem>, <chem>LaLuO3</chem>, <chem>LaO3Sc</chem>, <chem>LaO3Y</chem>, <chem>LaO9Ta3</chem>, <chem>LaPPt</chem>, <chem>LaPS</chem>, <chem>LaRbS4Si</chem>, <chem>LaS2</chem>, <chem>LaSbTe</chem>, <chem>La2O2S3Sn</chem>, <chem>La2O5Ti</chem>, <chem>La2S3</chem>, <chem>La2S5Th</chem>, <chem>La2S5U</chem>, <chem>La2S5Zr</chem>, <chem>La2Se5Th</chem>, <chem>La2Se5U</chem>, <chem>La2Se5Zr</chem>, <chem>La3NS3</chem>, <chem>La3NbO7</chem>, <chem>La4N2Te3</chem>, <chem>Li12Si7</chem>, <chem>LiMgN</chem>, <chem>LiNaSe</chem>, <chem>LiNaTe</chem>, <chem>LiORb</chem>, <chem>LiO4ScSi</chem>, <chem>LiSbSr</chem>, <chem>Li2O4U</chem>, <chem>Li2O7S2</chem>, <chem>Li2O7Se2</chem>, <chem>Li2S</chem>, <chem>Li3NaSi6</chem>, <chem>Li4S4Sn</chem>, <chem>Li4Se4Sn</chem>, <chem>Lu2PbS4</chem>, <chem>Lu2S4Sr</chem>, <chem>Lu2S4Zn</chem>, <chem>Lu2Se4Sr</chem>, <chem>Lu5Sb3</chem>, <chem>MgO3Se</chem>, <chem>MgO3Si</chem>, <chem>MgO4S</chem>, <chem>MgO4Se</chem>, <chem>MgO6Pb2W</chem>, <chem>MgPbSr</chem>, <chem>MgPd2</chem>, <chem>MgSiSr</chem>, <chem>MgSi2Sr</chem>, <chem>MgSnSr</chem>, <chem>Mg2O4Si</chem>, <chem>Mg2Pb</chem>, <chem>Mg2S4Si</chem>, <chem>Mg2S4Sn</chem>, <chem>Mg2Se4Si</chem>, <chem>Mg2Se4Sn</chem>, <chem>Mg2Si</chem>, <chem>MoO3</chem>, <chem>MoO4Rb2</chem>, <chem>MoPt3Si4</chem>, <chem>MoRb2S4</chem>, <chem>MoRb2Se4</chem>, <chem>MoSiZr</chem>, <chem>Mo3Sc2Si4</chem>, <chem>Mo4P3</chem>, <chem>NNa3</chem>, <chem>N3TaTh</chem>, <chem>N4Si3</chem>, <chem>N4Zr3</chem>, <chem>N5Ta3</chem>, <chem>Na</chem>, <chem>NaNbO3</chem>, <chem>NaO3Sb</chem>, <chem>NaO3Ta</chem>, <chem>NaO6ScSe2</chem>, <chem>NaP5</chem>, <chem>Na2S</chem>, <chem>Na2S5</chem>, <chem>Na3O2Tl</chem>, <chem>Na4Se4Si</chem>, <chem>NbPZr</chem>, <chem>NbRb3S4</chem>, <chem>Nb5P3</chem>, <chem>O14Rb3Ta5</chem>, <chem>OSiSr3</chem>, <chem>O2Pb</chem>, <chem>O2Sn</chem>, <chem>O2SrZn</chem>, <chem>O2Te</chem>, <chem>O2Th</chem>, <chem>O2Ti</chem>, <chem>O2W</chem>, <chem>O2Zr</chem>, <chem>O3PbRb2</chem>, <chem>O3PbS</chem>, <chem>O3PbSr</chem>, <chem>O3ScY</chem>, <chem>O3SeSr</chem>, <chem>O3SeZn</chem>, <chem>O3SnSr</chem>, <chem>O3SnTl2</chem>, <chem>O3SrZr</chem>, <chem>O3Ti2</chem>, <chem>O3W</chem>, <chem>O3Y2</chem>, <chem>O4PbS</chem>, <chem>O4Rb2S</chem>, <chem>O4Rb2Se</chem>, <chem>O4SSn</chem>, <chem>O4SSr</chem>, <chem>O4STl2</chem>, <chem>O4SZn</chem>, <chem>O4SeTl2</chem>, <chem>O4SiSr2</chem>, <chem>O4SiZn2</chem>, <chem>O4SrTl2</chem>, <chem>O4SrY2</chem>, <chem>O5P2</chem>, <chem>O5STi</chem>, <chem>O5TiY2</chem>, <chem>O6RbSe2Y</chem>, <chem>O6RbTe2Y</chem>, <chem>O7Si2Y2</chem>, <chem>P14PbZn</chem>, <chem>PPbRbS4</chem>, <chem>PPbS4Tl</chem>, <chem>PPtSc</chem>, <chem>PRb3S4</chem>, <chem>PSY</chem>, <chem>PS4SrTl</chem>, <chem>PS4Tl3</chem>, <chem>PSe3</chem>, <chem>PSe4Tl3</chem>, <chem>P2Th</chem>, <chem>P2Ti</chem>, <chem>P2Zr</chem>, <chem>P3Re</chem>, <chem>P3Ta5</chem>, <chem>P4S3</chem>, <chem>PbS</chem>, <chem>PbS3Sn</chem>, <chem>PbS3Zr</chem>, <chem>PbS4Sc2</chem>, <chem>PbS5U2</chem>, <chem>PbSc2Se4</chem>, <chem>PbSe</chem>, <chem>PbSe5U2</chem>, <chem>PbSr2</chem>, <chem>PbTe</chem>, <chem>Pb4Se4</chem>, <chem>Pb4Sr5</chem>, <chem>PdSc6Te2</chem>, <chem>PdSe3U</chem>, <chem>PdSi</chem>, <chem>PdSiTi</chem>, <chem>PdSiU</chem>, <chem>PdSiZr</chem>, <chem>PdSn</chem>, <chem>PdTe2Y6</chem>, <chem>PdTh</chem>, <chem>Pd2Sn</chem>, <chem>Pd2SnU</chem></p>
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Part 9 of all the predicted materials with band crossings from **Cases 1 or 2:**

62	Pd <sub>2</sub> Zn, Pd <sub>3</sub> Si, Pd <sub>3</sub> Ta <sub>2</sub> Te <sub>5</sub> , Pd <sub>9</sub> Si <sub>2</sub> , PtSc <sub>2</sub> , PtSi, PtSiTi, PtSiZr, PtSnSr, PtY <sub>2</sub> , Pt <sub>3</sub> Si, Pt <sub>3</sub> Sr <sub>7</sub> , Pt <sub>4</sub> Sr <sub>5</sub> , RbSb <sub>3</sub> Se <sub>5</sub> , Rb <sub>2</sub> S, Rb <sub>2</sub> S <sub>4</sub> W, Rb <sub>2</sub> Se <sub>4</sub> W, Rb <sub>2</sub> Te, Rb <sub>2</sub> Te <sub>3</sub> , Rb <sub>3</sub> S <sub>4</sub> Sb, Rb <sub>3</sub> S <sub>4</sub> Ta, Rb <sub>3</sub> SbSe <sub>4</sub> , SSeU, SSn, STeU, S <sub>2</sub> Th, S <sub>2</sub> Ti, S <sub>2</sub> U, S <sub>3</sub> Sb <sub>2</sub> , S <sub>3</sub> SnSr, S <sub>3</sub> SnZr, S <sub>3</sub> Sn <sub>2</sub> , S <sub>3</sub> SrZr, S <sub>3</sub> Sr <sub>2</sub> Zn, S <sub>3</sub> TaTl, S <sub>3</sub> TeTl <sub>2</sub> , S <sub>3</sub> Th <sub>2</sub> , S <sub>3</sub> U <sub>2</sub> , S <sub>3</sub> Y <sub>2</sub> , S <sub>4</sub> Sc <sub>2</sub> Sr, S <sub>4</sub> SrY <sub>2</sub> , S <sub>4</sub> Y <sub>2</sub> Zn, S <sub>5</sub> Sb <sub>2</sub> Sn <sub>2</sub> , S <sub>5</sub> TiU <sub>2</sub> , S <sub>5</sub> U <sub>3</sub> , S <sub>5</sub> Y <sub>2</sub> Zr, Sb <sub>2</sub> Se <sub>3</sub> , Sb <sub>2</sub> SrZn, Sb <sub>3</sub> Sc <sub>5</sub> , Sb <sub>4</sub> Sn <sub>3</sub> Sr, Sc <sub>2</sub> Si <sub>4</sub> W <sub>3</sub> , Sc <sub>2</sub> SrTe <sub>4</sub> , Sc <sub>2</sub> Te, SeSn, SeTeU, SeTi, SeTi <sub>2</sub> , Se <sub>2</sub> Th, Se <sub>2</sub> U, Se <sub>3</sub> SnTl <sub>2</sub> , Se <sub>3</sub> SrZr, Se <sub>3</sub> TaTl, Se <sub>3</sub> Th <sub>2</sub> , Se <sub>3</sub> U <sub>2</sub> , Se <sub>4</sub> SrY <sub>2</sub> , Se <sub>5</sub> U <sub>3</sub> , SiSr, SiSr <sub>2</sub> , SiTh, SiU, SiZr, SnSr <sub>2</sub> , SnTe, SnTe <sub>3</sub> Tl <sub>2</sub> , Sn <sub>4</sub> Th <sub>5</sub> , SrZn, SrZn <sub>5</sub> , TeZr, TeZr <sub>2</sub> , Te <sub>3</sub> U <sub>2</sub> , Te <sub>5</sub> U, Te <sub>5</sub> U <sub>3</sub> ,
63	Ag <sub>10</sub> Br <sub>3</sub> Te <sub>4</sub> , AgAuBa <sub>4</sub> O <sub>6</sub> , AgBaLaSe <sub>3</sub> , AgBaSe <sub>3</sub> Y, AgBaTe <sub>3</sub> Y, AgBiCl <sub>2</sub> S, AgBr <sub>2</sub> Cs, AgCl, AgCl <sub>2</sub> Cs, AgCsS <sub>3</sub> U, AgCsSe <sub>3</sub> U, AgCsTe <sub>3</sub> U, AgK <sub>2</sub> P, AgNa <sub>2</sub> Sb, AgNbO <sub>3</sub> , AgRbS <sub>3</sub> U, AgRbSe <sub>3</sub> U, AgS <sub>3</sub> Ta, Ag <sub>2</sub> Si, Ag <sub>3</sub> BrS, AlB-Mo, AlBW, AlCl <sub>8</sub> Nb, AlF <sub>3</sub> , AlF <sub>4</sub> Na, AlF <sub>5</sub> Tl <sub>2</sub> , AlGeLu, AlGeSc, AlHf <sub>3</sub> N, AlLa, AlLuSi, AlN, AlN <sub>2</sub> Zr <sub>3</sub> , AlSc, AlSiY, AlY, Al <sub>2</sub> BaSi <sub>2</sub> , Al <sub>2</sub> GeLa <sub>2</sub> , Al <sub>2</sub> MgO <sub>4</sub> , Al <sub>2</sub> O <sub>5</sub> Ti, Al <sub>4</sub> Mg <sub>19</sub> Zn <sub>15</sub> , AsAuNa <sub>2</sub> , AsBiMg <sub>2</sub> O <sub>6</sub> , AsIn, As <sub>2</sub> BaPd, As <sub>2</sub> BaPt, As <sub>2</sub> Cs <sub>2</sub> Pd, As <sub>2</sub> K <sub>2</sub> Pd, As <sub>2</sub> K <sub>2</sub> Pt, As <sub>2</sub> PtRb <sub>2</sub> , As <sub>3</sub> Nb <sub>4</sub> , As <sub>4</sub> Cd <sub>5</sub> Rb <sub>2</sub> , As <sub>4</sub> K <sub>2</sub> Zn <sub>5</sub> , As <sub>4</sub> Rb <sub>2</sub> Zn <sub>5</sub> , As <sub>6</sub> Ba <sub>4</sub> Cd <sub>3</sub> Li <sub>2</sub> , AuBiK <sub>2</sub> , AuBiNa <sub>2</sub> , AuCa <sub>2</sub> N, AuClTe <sub>2</sub> , AuCsS, AuCsSe, AuCsSe <sub>3</sub> U, AuCsTe <sub>3</sub> U, AuIn <sub>2</sub> Na, AuKS, AuKSe, AuK <sub>2</sub> P, AuK <sub>2</sub> Sb, AuLa, AuNS <sub>2</sub> , AuNaO <sub>2</sub> , AuNa <sub>2</sub> Sb, AuO <sub>2</sub> Rb, AuRbS, AuRbSe, AuRbSe, AuRbSe <sub>3</sub> U, AuRbTe <sub>3</sub> U, AuY, Au <sub>2</sub> P <sub>2</sub> Pb, Au <sub>3</sub> Mg, BF <sub>4</sub> Na, BNU, BNb, BO <sub>3</sub> Y, BTa, B <sub>2</sub> BaGa <sub>2</sub> O <sub>7</sub> , B <sub>2</sub> Li <sub>2</sub> S <sub>5</sub> , B <sub>4</sub> O <sub>7</sub> Zn, B <sub>7</sub> WY <sub>3</sub> , BaBiClO <sub>2</sub> , BaBiO <sub>2</sub> , BaCd <sub>2</sub> Pt, BaClO <sub>2</sub> Sb, BaF <sub>4</sub> Mg, BaGe, BaIn, BaIn <sub>2</sub> Pt, BaLa <sub>2</sub> O <sub>10</sub> Ti <sub>3</sub> , BaOSzn, BaO <sub>6</sub> Te <sub>2</sub> , BaO <sub>8</sub> Si <sub>2</sub> U, BaPb, BaPdS <sub>2</sub> , BaPdSb <sub>2</sub> , BaSi, BaSi <sub>6</sub> , BaSn, BaZn <sub>5</sub> , Ba <sub>3</sub> Cl <sub>2</sub> O <sub>5</sub> W, Ba <sub>3</sub> Ge <sub>5</sub> , Ba <sub>3</sub> Pb <sub>5</sub> , Ba <sub>3</sub> Sn <sub>5</sub> , Ba <sub>4</sub> Cd <sub>3</sub> Li <sub>2</sub> P <sub>6</sub> , Ba <sub>5</sub> Cd <sub>2</sub> FSb <sub>5</sub> , BeHf, BePd <sub>3</sub> , BiBrO <sub>2</sub> Sr, BiClO <sub>2</sub> Pb, BiClO <sub>2</sub> Pb, BiClO <sub>2</sub> Sr, BiO <sub>2</sub> Sr, BiO <sub>4</sub> Re, Bi <sub>2</sub> Ca, Bi <sub>2</sub> Cs <sub>2</sub> Pd, Bi <sub>2</sub> Cs <sub>2</sub> Pt, BrIn, BrLaO <sub>7</sub> Pb <sub>6</sub> , BrO <sub>4</sub> Y <sub>3</sub> , BrTl, Br <sub>2</sub> LiRb, Br <sub>2</sub> O <sub>11</sub> Te <sub>6</sub> , Br <sub>3</sub> CaIn, Br <sub>6</sub> Mo <sub>6</sub> S <sub>3</sub> , CAgNO, CB <sub>3</sub> Nb <sub>3</sub> , C <sub>2</sub> BF <sub>2</sub> LiO <sub>4</sub> , C <sub>3</sub> BLu <sub>3</sub> , C <sub>56</sub> Cl <sub>10</sub> , C <sub>70</sub> , CaGe, CaIn <sub>2</sub> Pd, CaIn <sub>2</sub> Pt, CaIn <sub>4</sub> Pd, CaO <sub>3</sub> Pt, CaO <sub>4</sub> S, CaO <sub>4</sub> Ti <sub>2</sub> , CaO <sub>4</sub> Ti <sub>2</sub> , CaO <sub>4</sub> Tl <sub>2</sub> , CaPdSn <sub>2</sub> , CaSi, CaSn, CaZn, Ca <sub>2</sub> InN, Ca <sub>2</sub> Sn <sub>6</sub> Zn <sub>3</sub> , Ca <sub>2</sub> Zn, CdCsLaTe <sub>3</sub> , CdCsLuTe <sub>3</sub> , CdCsSe <sub>3</sub> Y, CdF <sub>7</sub> RbZr, CdF <sub>7</sub> TlZr, CdO <sub>4</sub> S, CdTe, Cd <sub>2</sub> FSb <sub>5</sub> Sr <sub>5</sub> , Cd <sub>2</sub> PdSr, Cl <sub>12</sub> Rb <sub>3</sub> Re <sub>3</sub> , ClCsO <sub>2</sub> , ClIn, ClKO <sub>2</sub> , ClNaO <sub>4</sub> , ClO <sub>2</sub> PbSb, ClO <sub>2</sub> Rb, ClTl, Cl <sub>2</sub> LiRb, Cl <sub>2</sub> MoO <sub>5</sub> Pb <sub>3</sub> , Cl <sub>2</sub> O <sub>11</sub> Te <sub>6</sub> , Cl <sub>2</sub> O <sub>5</sub> Pb <sub>3</sub> W, Cl <sub>3</sub> Cs <sub>2</sub> Li, Cl <sub>3</sub> F <sub>10</sub> K <sub>3</sub> Sn <sub>5</sub> , Cl <sub>4</sub> CsLi <sub>3</sub> , Cl <sub>4</sub> Cs <sub>2</sub> Pd, Cl <sub>4</sub> Cs <sub>2</sub> Pt, CsHgLaSe <sub>3</sub> , CsHgSe <sub>3</sub> Y, CsLaTe <sub>3</sub> Zn, CsNaO <sub>3</sub> Ti, CsScSe <sub>5</sub> U, CsSe <sub>3</sub> YZn, CsTe <sub>3</sub> YZn, Cs <sub>2</sub> F <sub>4</sub> OTe, Cs <sub>2</sub> O <sub>3</sub> Pb, Cs <sub>2</sub> O <sub>3</sub> Zr, Cs <sub>2</sub> P <sub>2</sub> Pt, Cs <sub>2</sub> PdSb <sub>2</sub> , Cs <sub>2</sub> PtSb <sub>2</sub> , Cs <sub>2</sub> Se <sub>3</sub> Zr, Cs <sub>2</sub> Te <sub>5</sub> , Cs <sub>3</sub> NaPb <sub>4</sub> , F <sub>10</sub> Pb <sub>3</sub> Zr, F <sub>14</sub> I <sub>2</sub> Pb <sub>8</sub> , F <sub>2</sub> INaO <sub>2</sub> , F <sub>2</sub> O <sub>2</sub> Xe, F <sub>3</sub> ISn <sub>2</sub> , F <sub>3</sub> MgNa, F <sub>4</sub> K <sub>2</sub> OTe, F <sub>4</sub> MgSr, F <sub>5</sub> K <sub>2</sub> Sb, F <sub>6</sub> K <sub>2</sub> Zr, F <sub>6</sub> Rb <sub>2</sub> U, Ga, Ga <sub>13</sub> K <sub>3</sub> , GaLa, GaLu, GaSc, GaU, GaY, GeLa, GeLi <sub>4</sub> O <sub>4</sub> , GeMgO <sub>3</sub> , GeNa <sub>2</sub> Zn, GeS, Ge <sub>2</sub> Hf, Ge <sub>2</sub> Pt <sub>3</sub> , Ge <sub>2</sub> Th, Ge <sub>2</sub> U, Ge <sub>3</sub> La <sub>2</sub> Li <sub>2</sub> , Ge <sub>4</sub> Na <sub>4</sub> S <sub>10</sub> , Ge <sub>4</sub> Na <sub>4</sub> Se <sub>10</sub> , Ge <sub>6</sub> La <sub>2</sub> Zn <sub>3</sub> , Ge <sub>8</sub> Na <sub>15</sub> PSn, HfO <sub>3</sub> Sr, HfPd, HfPt, HfSi <sub>2</sub> , HfTe <sub>5</sub> , HgNa, HgNa <sub>2</sub> Pb, HgTe, IIn, IK <sub>4</sub> P <sub>21</sub> , IP <sub>21</sub> Rb <sub>4</sub> , ITl, I <sub>3</sub> La, I <sub>3</sub> PbTl, InSb, In <sub>2</sub> PdSr, In <sub>2</sub> PtSr, In <sub>4</sub> PbSr <sub>3</sub> , In <sub>4</sub> PdSr, In <sub>4</sub> PtSr, In <sub>5</sub> La <sub>3</sub> , In <sub>5</sub> Y <sub>3</sub> , KNb <sub>3</sub> O <sub>8</sub> ,

Part 10 of all the predicted materials with band crossings from **Cases 1 or 2**:

	K <sub>2</sub> O <sub>3</sub> Ti, K <sub>2</sub> P <sub>2</sub> Pd, LaLiSn <sub>2</sub> , LaSi, La <sub>2</sub> Li <sub>2</sub> Si <sub>3</sub> , La <sub>2</sub> PbZn <sub>5</sub> , La <sub>2</sub> SnZn <sub>5</sub> , La <sub>2</sub> Te <sub>5</sub> , La <sub>3</sub> NbO <sub>7</sub> , La <sub>3</sub> O <sub>7</sub> Sb, La <sub>3</sub> O <sub>7</sub> Ta, La <sub>3</sub> Tl <sub>5</sub> , LiLuSn <sub>2</sub> , Li <sub>2</sub> Nb <sub>2</sub> O <sub>7</sub> Sr, Li <sub>2</sub> O <sub>4</sub> S, Li <sub>2</sub> O <sub>7</sub> SrTa <sub>2</sub> , Li <sub>4</sub> O <sub>4</sub> Pb, Li <sub>4</sub> O <sub>4</sub> Ti, Lu <sub>3</sub> Tl <sub>5</sub> , MgO <sub>3</sub> Si, MgO <sub>4</sub> S, MgO <sub>4</sub> Se, Mg <sub>2</sub> PdSr, MoNNa <sub>5</sub> O <sub>4</sub> , Mo <sub>9</sub> Se <sub>11</sub> , NO <sub>2</sub> SiY, N <sub>3</sub> TaTh, N <sub>5</sub> Ta <sub>3</sub> , NaNbO <sub>3</sub> , NaO <sub>3</sub> Ta, Na <sub>2</sub> O <sub>4</sub> S, Na <sub>2</sub> S <sub>5</sub> Si <sub>2</sub> , Na <sub>2</sub> Tl <sub>2</sub> , Na <sub>4</sub> S <sub>10</sub> Si <sub>4</sub> , Na <sub>4</sub> Se <sub>10</sub> Si <sub>4</sub> , Na <sub>5</sub> Sn <sub>13</sub> , Na <sub>6</sub> O <sub>5</sub> Pb, O <sub>14</sub> Si <sub>4</sub> Sr <sub>2</sub> Ti <sub>2</sub> , O <sub>2</sub> Te, O <sub>3</sub> SrZr, O <sub>4</sub> SiTi, O <sub>5</sub> Ti <sub>3</sub> , O <sub>6</sub> Pb <sub>3</sub> S, O <sub>7</sub> SbY <sub>3</sub> , O <sub>7</sub> Sn <sub>2</sub> Sr <sub>3</sub> , O <sub>7</sub> Sr <sub>2</sub> Ta <sub>2</sub> , O <sub>7</sub> TaY <sub>3</sub> , O <sub>8</sub> U <sub>3</sub> , PbS, PbSr, Pb <sub>4</sub> Se <sub>4</sub> , PdSr, PdSrTl <sub>2</sub> , PdZr, Pd <sub>3</sub> Te <sub>2</sub> , Pd <sub>3</sub> Ti <sub>2</sub> , PtTh, PtU, PtZr, SiZr, Si <sub>24</sub> , Si <sub>2</sub> Ti, Si <sub>2</sub> Zr, Si <sub>6</sub> Sr, SnSr, SnTi <sub>3</sub> , Sn <sub>2</sub> Th, Sn <sub>4</sub> Sr, Sn <sub>5</sub> Sr <sub>3</sub> , TeZn, Te <sub>3</sub> U, Te <sub>5</sub> Zr, TiZn <sub>16</sub> , Tl <sub>5</sub> Y <sub>3</sub> , U,
63	AgNO <sub>3</sub> , Ag <sub>2</sub> Cl <sub>4</sub> Pd, Ag <sub>2</sub> HfS <sub>3</sub> , AlBa <sub>3</sub> Sb <sub>3</sub> , AlLi, AlLiNa <sub>2</sub> P <sub>2</sub> , AlSb <sub>3</sub> Sr <sub>3</sub> , As, AsHg <sub>4</sub> I <sub>5</sub> , As <sub>2</sub> GaK <sub>2</sub> Li, As <sub>2</sub> GaLiNa <sub>2</sub> , As <sub>2</sub> InK <sub>2</sub> Li, As <sub>3</sub> In <sub>2</sub> K <sub>3</sub> , As <sub>6</sub> K <sub>6</sub> Na <sub>4</sub> Sn <sub>2</sub> , Au <sub>3</sub> Zn, B <sub>12</sub> Li <sub>2</sub> Si <sub>2</sub> , B <sub>2</sub> BaSe <sub>6</sub> , B <sub>2</sub> Br <sub>4</sub> Cl <sub>6</sub> N <sub>2</sub> P <sub>2</sub> , BaGe <sub>2</sub> O <sub>5</sub> , Ba <sub>2</sub> Si, BaO <sub>14</sub> Sn <sub>4</sub> U <sub>3</sub> , Ba <sub>2</sub> Bi <sub>4</sub> Cd <sub>3</sub> , Ba <sub>2</sub> Ca <sub>2</sub> Sn <sub>6</sub> , Ba <sub>2</sub> F <sub>6</sub> Pd, Ba <sub>2</sub> Ge <sub>4</sub> Pd <sub>5</sub> , Ba <sub>4</sub> O <sub>10</sub> PtTi <sub>2</sub> , Ba <sub>4</sub> OP <sub>2</sub> , Ba <sub>5</sub> P <sub>4</sub> , Ba <sub>5</sub> Sb <sub>4</sub> , Ba <sub>6</sub> Ga <sub>2</sub> P <sub>6</sub> , BiSn, Bi <sub>2</sub> MoO <sub>6</sub> , Bi <sub>5</sub> BrO <sub>7</sub> , Br, Br <sub>12</sub> Mo <sub>6</sub> , Br <sub>12</sub> W <sub>6</sub> , Br <sub>14</sub> Ta <sub>6</sub> , Br <sub>16</sub> W <sub>6</sub> , Br <sub>2</sub> , CCl <sub>14</sub> Ti <sub>6</sub> , CCl <sub>14</sub> Zr <sub>6</sub> , Cl <sub>14</sub> Zr <sub>6</sub> , CO <sub>2</sub> , CS <sub>2</sub> , CSe <sub>2</sub> , C <sub>2</sub> B <sub>2</sub> Mg, C <sub>2</sub> N <sub>2</sub> Se, Ca, CaO <sub>4</sub> Se, CaO <sub>4</sub> W, Ca <sub>2</sub> N <sub>3</sub> P, Ca <sub>5</sub> Ga <sub>2</sub> N <sub>4</sub> , Ca <sub>5</sub> O <sub>14</sub> Te <sub>3</sub> , CdClIO <sub>3</sub> , Cl, Cl <sub>12</sub> Mo <sub>6</sub> , Cl <sub>14</sub> Nb <sub>6</sub> , Cl <sub>16</sub> Li <sub>2</sub> Nb <sub>6</sub> , Cl <sub>2</sub> , Cs, Cs <sub>3</sub> Na <sub>2</sub> P <sub>3</sub> Sn, Cs <sub>4</sub> F <sub>10</sub> Mg <sub>3</sub> , Cs <sub>4</sub> F <sub>10</sub> Zn <sub>3</sub> , F <sub>3</sub> Na <sub>2</sub> O <sub>4</sub> SSb, Ga, Ge, Ge <sub>2</sub> Sn <sub>2</sub> , HgO <sub>4</sub> W, I, I <sub>14</sub> Ta <sub>6</sub> , I <sub>2</sub> , I <sub>2</sub> Mo, InK <sub>2</sub> NaSb <sub>2</sub> , In <sub>9</sub> KNa <sub>3</sub> , K, KLiO, KTi, K <sub>2</sub> O <sub>2</sub> , K <sub>3</sub> Na <sub>2</sub> P <sub>3</sub> Sn, K <sub>4</sub> Sn <sub>2</sub> Te <sub>6</sub> , LaS, La <sub>2</sub> O <sub>2</sub> S <sub>2</sub> , Li, LiTl, Mo <sub>2</sub> Na <sub>2</sub> O <sub>7</sub> , Na <sub>2</sub> O <sub>7</sub> W <sub>2</sub> , Na <sub>4</sub> P <sub>2</sub> Se <sub>6</sub> , NbP <sub>2</sub> S <sub>8</sub> , O <sub>2</sub> Si, O <sub>3</sub> Rb <sub>2</sub> Ti, O <sub>4</sub> PbW, O <sub>4</sub> SnSr <sub>2</sub> , O <sub>4</sub> WZn, O <sub>5</sub> Si <sub>2</sub> Sr, P, PdSn <sub>3</sub> , Pd <sub>8</sub> Sn <sub>24</sub> , Rb, Sn <sub>3</sub> Ti <sub>2</sub> ,
64	Al <sub>2</sub> PbS <sub>4</sub> , Al <sub>2</sub> S <sub>4</sub> Sr, Al <sub>2</sub> Se <sub>4</sub> Sr, BaGa <sub>2</sub> Se <sub>4</sub> , BaIn <sub>2</sub> Te <sub>4</sub> , Ba <sub>3</sub> S <sub>7</sub> Zr <sub>2</sub> , CaGa <sub>2</sub> S <sub>4</sub> , Ga <sub>2</sub> PbSe <sub>4</sub> , Ga <sub>2</sub> S <sub>4</sub> Sr, Ga <sub>2</sub> Se <sub>4</sub> Sr, Ga <sub>2</sub> SrTe <sub>4</sub> , I <sub>3</sub> Th, In <sub>2</sub> SrTe <sub>4</sub> ,
66	AgClO <sub>2</sub> , AlB <sub>2</sub> CaO <sub>7</sub> , Al <sub>4</sub> O <sub>7</sub> Sr, Au <sub>2</sub> Cd <sub>2</sub> Cs <sub>2</sub> S <sub>4</sub> , BaF <sub>6</sub> Zr, C, ClFOPb <sub>2</sub> , Cl <sub>9</sub> PSn, F <sub>3</sub> La, F <sub>6</sub> PaRb, F <sub>6</sub> PbZr, OPb,
67	Al <sub>2</sub> F <sub>16</sub> Sr <sub>5</sub> , AuNaS, CaCl <sub>2</sub> O <sub>4</sub> , Cl <sub>2</sub> O <sub>4</sub> Pb, Cl <sub>2</sub> O <sub>4</sub> Sr, K <sub>4</sub> Se <sub>8</sub> Sn <sub>3</sub> , O <sub>2</sub> Si, Pd <sub>4</sub> Sn <sub>16</sub> , PtSn <sub>4</sub> ,
70	AgCs <sub>2</sub> NbS <sub>4</sub> , AgCs <sub>2</sub> NbSe <sub>4</sub> , AgCs <sub>2</sub> S <sub>4</sub> Ta, AgK <sub>2</sub> NbS <sub>4</sub> , AgK <sub>2</sub> S <sub>4</sub> Ta, AgNbRb <sub>2</sub> S <sub>4</sub> , AgNbRb <sub>2</sub> Se <sub>4</sub> , AgRb <sub>2</sub> S <sub>4</sub> Ta, Ag <sub>2</sub> Ba <sub>4</sub> Si <sub>6</sub> , Ag <sub>2</sub> GeK <sub>2</sub> Se <sub>4</sub> , Ag <sub>2</sub> O <sub>4</sub> S, Ag <sub>2</sub> O <sub>4</sub> Se, Al <sub>2</sub> CaS <sub>4</sub> , Al <sub>2</sub> S <sub>4</sub> Sr, AsMoO <sub>6</sub> Rb, As <sub>2</sub> Na <sub>2</sub> O <sub>8</sub> Th, AuLiS, Au <sub>2</sub> BaP <sub>4</sub> , Au <sub>2</sub> Cs <sub>2</sub> S <sub>4</sub> Sn, B <sub>2</sub> BaBe <sub>2</sub> O <sub>6</sub> , BaCl <sub>2</sub> O <sub>8</sub> , Ba <sub>2</sub> CaN <sub>4</sub> W, Ba <sub>3</sub> GeI <sub>2</sub> , Ba <sub>3</sub> I <sub>2</sub> Si, Ba <sub>4</sub> Ge <sub>6</sub> Li <sub>2</sub> , Ba <sub>4</sub> Li <sub>2</sub> Si <sub>6</sub> , Ba <sub>4</sub> MgN <sub>6</sub> Si <sub>2</sub> , BiCa <sub>2</sub> Na <sub>3</sub> O <sub>6</sub> , CaGa <sub>2</sub> S <sub>4</sub> , Ca <sub>2</sub> Na <sub>3</sub> O <sub>6</sub> Ta, Cd <sub>2</sub> O <sub>4</sub> Si, CsTl, FInO, Ga <sub>2</sub> PbS <sub>4</sub> , Ga <sub>2</sub> PbSe <sub>4</sub> , Ga <sub>2</sub> S <sub>4</sub> Sr, Ga <sub>4</sub> LaNaSes, GeHg <sub>2</sub> O <sub>4</sub> , Ge <sub>2</sub> Ti, Ge <sub>6</sub> Li <sub>2</sub> Sr <sub>4</sub> , In <sub>2</sub> S <sub>4</sub> Sr, In <sub>2</sub> Se <sub>4</sub> Sr, K <sub>2</sub> Pd <sub>3</sub> S <sub>4</sub> , K <sub>4</sub> P <sub>6</sub> , Li <sub>2</sub> Si <sub>6</sub> Sr <sub>4</sub> , Lu <sub>2</sub> Te <sub>3</sub> , MoNa <sub>2</sub> O <sub>4</sub> , Na <sub>2</sub> O <sub>3</sub> Pt, Na <sub>2</sub> O <sub>4</sub> S, Na <sub>2</sub> O <sub>4</sub> Se, NbSn <sub>2</sub> , Nb <sub>2</sub> O <sub>10</sub> TiU, O <sub>2</sub> Si, O <sub>3</sub> U, P <sub>2</sub> S <sub>7</sub> U, Pd <sub>3</sub> Rb <sub>2</sub> S <sub>4</sub> , Pd <sub>3</sub> Rb <sub>2</sub> Se <sub>4</sub> , Rb, S <sub>3</sub> Sc <sub>2</sub> , S <sub>8</sub> , SbSnTi, Sc <sub>2</sub> Te <sub>3</sub> , Se <sub>3</sub> Y <sub>2</sub> , Si <sub>2</sub> Ti, Sn <sub>2</sub> Ta, Sn <sub>2</sub> Zr, Te <sub>3</sub> Y <sub>2</sub> ,
72	AgN <sub>3</sub> , AgNa <sub>3</sub> O <sub>2</sub> , AgNa <sub>3</sub> S <sub>2</sub> , AgNb <sub>3</sub> O <sub>8</sub> , Ag <sub>3</sub> LiO <sub>2</sub> , Ag <sub>3</sub> NaO <sub>2</sub> , AlAs <sub>2</sub> K <sub>2</sub> Na, AlAs <sub>2</sub> Na <sub>3</sub> , AlK <sub>2</sub> LiP <sub>2</sub> , AlK <sub>2</sub> NaP <sub>2</sub> , AlNa <sub>3</sub> P <sub>2</sub> , As <sub>2</sub> Ba <sub>2</sub> Zn, As <sub>2</sub> Cs <sub>2</sub> Si, As <sub>2</sub> Cs <sub>2</sub> Sn, As <sub>2</sub> GaK <sub>2</sub> Na, As <sub>2</sub> GeK <sub>2</sub> , As <sub>2</sub> InK <sub>2</sub> Na, As <sub>2</sub> K <sub>2</sub> Si, As <sub>2</sub> Rb <sub>2</sub> Si, AuKSe <sub>5</sub> , AuKSe <sub>5</sub> ,

Part 11 of all the predicted materials with band crossings from **Cases 1 or 2**:

	<chem>AuLi3S2</chem> , <chem>Au4CdK2S4</chem> , <chem>Ba2Bi2Zn</chem> , <chem>Ba2Br2O</chem> , <chem>Ba2I2O</chem> , <chem>Ba2Sb2Zn</chem> , <chem>BeBr2</chem> , <chem>BeCl2</chem> , <chem>BeI2</chem> , <chem>BiLiO2</chem> , <chem>Br2Hg5O4</chem> , <chem>Cd3Cs2Te4</chem> , <chem>Cl2Hg5O4</chem> , <chem>Cl3La2N</chem> , <chem>Cl6Cs2Pd2</chem> , <chem>Cs2GaLi3O4</chem> , <chem>Cs2Hg3S4</chem> , <chem>Cs2Hg3Se4</chem> , <chem>Cs2P2Si</chem> , <chem>Cs2S4Zn3</chem> , <chem>F11LaZr2</chem> , <chem>GaK2NaP2</chem> , <chem>Ge2Mg5</chem> , <chem>Ge5Ti6</chem> , <chem>Hg2O3Se</chem> , <chem>I2OSr2</chem> , <chem>InK2NaP2</chem> , <chem>InK3P2</chem> , <chem>In2Mg5</chem> , <chem>K2O2Zn</chem> , <chem>K2P2Si</chem> , <chem>K2Te2Zn</chem> , <chem>MgO</chem> , <chem>Mg5Tl2</chem> , <chem>NaNb3O8</chem> , <chem>NaO8Ta3</chem> , <chem>Na2S2Zn</chem> , <chem>O2Si</chem> , <chem>Pb5Sc6</chem> , <chem>Pt3Sb2</chem> , <chem>Pt5Ti3</chem> , <chem>Rb2S4Zn3</chem> , <chem>S2Si</chem> , <chem>Se2Si</chem> ,
72	<chem>AlAs2Li3</chem> , <chem>Alli3P2</chem> , <chem>BiPS4</chem> , <chem>Bi3K3Na2Sn</chem> , <chem>Li4N3Ta</chem> ,
73	<chem>Ag2Ba</chem> , <chem>Ag2Ca</chem> , <chem>Ag2O7Te2</chem> , <chem>Ag2Sr</chem> , <chem>AlB14Li</chem> , <chem>AlF7MgNa2</chem> , <chem>AlF7Na2Zn</chem> , <chem>AllaO3</chem> , <chem>Al2Sr</chem> , <chem>Au2Ca</chem> , <chem>Au2Sr</chem> , <chem>Au5K3Pb</chem> , <chem>B15Na</chem> , <chem>B3Si</chem> , <chem>B7Mg</chem> , <chem>BaCd2</chem> , <chem>BaGe5</chem> , <chem>BaHg2</chem> , <chem>BaIn2</chem> , <chem>BaO3Pb</chem> , <chem>BaZn2</chem> , <chem>Ba2O7U2</chem> , <chem>Be2K2O11Si3Zn2</chem> , <chem>C2B12Mg</chem> , <chem>C2B13Li</chem> , <chem>CaCd2</chem> , <chem>CaO3Si</chem> , <chem>CaZn2</chem> , <chem>Ca2O7Sb2</chem> , <chem>Cd2Sr</chem> , <chem>CsF3MoO2</chem> , <chem>CsF5Pd2</chem> , <chem>F5Pd2Rb</chem> , <chem>Ge</chem> , <chem>HfO3Sr</chem> , <chem>Hg2Sr</chem> , <chem>Hg3I2S2</chem> , <chem>Hg3I2Se2</chem> , <chem>KNa2O15Si6Y</chem> , <chem>LaNb2O7Rb</chem> , <chem>MgO4U</chem> , <chem>Mg2O4Si</chem> , <chem>MoTi</chem> , <chem>Na2O7Te2</chem> , <chem>O2PbPd</chem> , <chem>O3SnSr</chem> , <chem>O3SrZr</chem> , <chem>O4SiZn2</chem> , <chem>O7Sb2Sr2</chem> , <chem>Si</chem> , <chem>Sr</chem> , <chem>SrZn2</chem> , <chem>Te</chem> ,
74	<chem>BO2Tl</chem> , <chem>Br5PbTl3</chem> , <chem>Cl5PbTl3</chem> , <chem>Cl8ISb</chem> , <chem>Cs3P7</chem> , <chem>Cs4Ge9</chem> , <chem>O3PbTe</chem> ,
76	<chem>AlF5Sr</chem> , <chem>BrCl14P3</chem> , <chem>Br4OW</chem> , <chem>Cl3F2Sb</chem> , <chem>Cl4OW</chem> ,
79	<chem>Ag3BiO3</chem> , <chem>AsNb</chem> , <chem>Ca11O24Re4</chem> , <chem>Cs5N10NaW4</chem> , <chem>Na2O12W3Zr</chem> , <chem>NbO2</chem> ,
80	<chem>As5BO20Pb6</chem> , <chem>Au2CaF12</chem> , <chem>B8Cd12Ge17O58</chem> , <chem>CO4Rb4</chem> , <chem>C2Ag10F8</chem> , <chem>GeSe2</chem> , <chem>I3NaOs</chem> , <chem>KMo4O6</chem> , <chem>P2S6Zr</chem> , <chem>Ta22</chem> , <chem>Ta30</chem> ,
81	<chem>AgI3O8</chem> , <chem>AgKO</chem> , <chem>Ag2HgI4</chem> , <chem>AlAsO4</chem> , <chem>AlO4P</chem> , <chem>Al2Be2Cl2Na8O24Si8</chem> , <chem>Al2CdS4</chem> , <chem>Al2CdSe4</chem> , <chem>Al2CdTe4</chem> , <chem>Al2HgS4</chem> , <chem>Al2HgSe4</chem> , <chem>Al2HgTe4</chem> , <chem>Al2Se4Zn</chem> , <chem>Al2Te4Zn</chem> , <chem>Al4Bi4Cl16S4</chem> , <chem>Al4Bi4Cl16Se4</chem> , <chem>Al4Bi4Cl16Te4</chem> , <chem>AsBO4</chem> , <chem>AsPd3</chem> , <chem>As4CsF13</chem> , <chem>Au2BaF8</chem> , <chem>BGeLiO4</chem> , <chem>BLiO4Si</chem> , <chem>BaBr2F8</chem> , <chem>BeO4S</chem> , <chem>Br16Re4Te8</chem> , <chem>CF2NO2P</chem> , <chem>CK4O4</chem> , <chem>CaF8HfLi2</chem> , <chem>CdGa2S4</chem> , <chem>CdGa2Se4</chem> , <chem>CdGa2Te4</chem> , <chem>CdIn2Se4</chem> , <chem>CdIn2Te4</chem> , <chem>CdTe4Tl2</chem> , <chem>Cl16Re4S4Te4</chem> , <chem>Cl16Re4Se4Te4</chem> , <chem>Cl16Re4Te8</chem> , <chem>Cl4FTa</chem> , <chem>F13KSb4</chem> , <chem>FK5La4O16Si4</chem> , <chem>FNa5O16Si4Y4</chem> , <chem>GaN5O14</chem> , <chem>Ga2HgS4</chem> , <chem>Ga2HgSe4</chem> , <chem>Ga2S4Zn</chem> , <chem>Ga2Se4Zn</chem> , <chem>Ga2Te4Zn</chem> , <chem>GeHg2Se4</chem> , <chem>GeSe2</chem> , <chem>GeTa3</chem> , <chem>GeTi3</chem> , <chem>Hf3Sb</chem> , <chem>HgIn2Se4</chem> , <chem>HgIn2Te4</chem> , <chem>Hg2Se4Sn</chem> , <chem>InPS4</chem> , <chem>In2Se4Zn</chem> , <chem>In2Te4Zn</chem> , <chem>LiPS4Zn</chem> , <chem>Mo3P</chem> , <chem>Nb9O25P</chem> , <chem>PW3</chem> , <chem>SbZr3</chem> , <chem>TeZr3</chem> , <chem>Te3Tl5</chem> ,
82	<chem>BiCl6Tl3</chem> , <chem>Cl6NaSb</chem> , <chem>Cs3I6La</chem> , <chem>F4Zr</chem> , <chem>La2O5Pd2</chem> , <chem>O8SrTe3</chem> , <chem>P2S6Th</chem> , <chem>P2S6U</chem> , <chem>P2S6Zr</chem> , <chem>PdS</chem> , <chem>PdSe</chem> , <chem>PtS</chem> ,
84	<chem>AgClO4Pb4</chem> , <chem>AgI</chem> , <chem>Ag7CsS4</chem> , <chem>Ag7RbS4</chem> , <chem>AsClNbO5Rb</chem> , <chem>AsCl2F3</chem> , <chem>As2Cl4F6</chem> , <chem>Bi4Cl14Se4</chem> , <chem>Br2Sr</chem> , <chem>Br9O4Pb8Tl</chem> , <chem>Cl4F6PSb</chem> , <chem>Cl5P</chem> , <chem>I4O12Zr</chem> , <chem>La9O5Sb5</chem> , <chem>P2U</chem> , <chem>Se2U</chem> ,
85	<chem>Ag4O4Si</chem> , <chem>AsZr3</chem> , <chem>As2O3</chem> , <chem>CK4O4</chem> , <chem>F3KOTe</chem> , <chem>GeNb3</chem> , <chem>GeTa3</chem> , <chem>ILiO3</chem> , <chem>Nb3Si</chem> , <chem>PZr3</chem> , <chem>SbY3</chem> , <chem>SiTa3</chem> ,
86	<chem>AlF6K3</chem> , <chem>Al3F19Pb5</chem> , <chem>Au4Ti</chem> , <chem>BBa2Cl17Zr6</chem> , <chem>BaF11LiZr2</chem> , <chem>Ba2CaO6W</chem> , <chem>Ba2O6TaY</chem> , <chem>BiF5</chem> , <chem>Br5Hg6S4Tl</chem> , <chem>Br5Hg6Se4Tl</chem> , <chem>Br6Rb2Te</chem> , <chem>C4Al4Th</chem> , <chem>CdO6Sr2W</chem> , <chem>Cl16Hg3Tl10</chem> , <chem>CsGe4Li12Na3O16</chem> , <chem>CsKLi12Na2O16Si4</chem> , <chem>F13KSb4</chem> , <chem>F6OXe2</chem> , <chem>F7IXe</chem> , <chem>GaO6SbSr2</chem> , <chem>GaO6Sr2Ta</chem> , <chem>Ga2Te5</chem> ,
87	

Part 12 of all the predicted materials with band crossings from **Cases 1 or 2**:

87	<chem>Hf5Te4</chem> , <chem>I12K4OTi4</chem> , <chem>InO6Sr2Ta</chem> , <chem>K5Te3</chem> , <chem>La2MoO5</chem> , <chem>Li12Na3O16RbSi4</chem> , <chem>Li4O5U</chem> , <chem>MgMoO6Sr2</chem> , <chem>MgO6ReSr2</chem> , <chem>MgO6Sr2W</chem> , <chem>MoO6Sr2Zn</chem> , <chem>O3PbTi</chem> , <chem>O5Ti4</chem> , <chem>O6Sr2TaY</chem> , <chem>O6Sr2TiZr</chem> , <chem>O6Sr2WZn</chem> , <chem>Se4Ti5</chem> , <chem>Te3Tl5</chem> , <chem>Te4Ti5</chem> , <chem>Te4Zr5</chem> ,
88	<chem>AgO</chem> , <chem>AsBiO4</chem> , <chem>AsCa2O12W2Y</chem> , <chem>Au2BaO4</chem> , <chem>Au2CaO4</chem> , <chem>Au2O4Sr</chem> , <chem>BaF11NaZr2</chem> , <chem>BaMoO4</chem> , <chem>BaO4W</chem> , <chem>BiF4Li</chem> , <chem>BrCsO4</chem> , <chem>Br4Th</chem> , <chem>Br6Rb2Sb</chem> , <chem>CaF4Zn</chem> , <chem>CaMg3N4Si</chem> , <chem>CaMoO4</chem> , <chem>CaO4Se</chem> , <chem>CaO4W</chem> , <chem>CdMoO4</chem> , <chem>Cl4KTl</chem> , <chem>Cl4SrZn</chem> , <chem>Cl4Th</chem> , <chem>Cl4Tl2</chem> , <chem>F4LiSc</chem> , <chem>F4LiY</chem> , <chem>F4SrZn</chem> , <chem>F7K3U</chem> , <chem>GeHfO4</chem> , <chem>GeLi</chem> , <chem>GeLi3NaO4</chem> , <chem>GeO4Th</chem> , <chem>GeO4U</chem> , <chem>GeO4Zr</chem> , <chem>Hg16Rb15</chem> , <chem>IInSe</chem> , <chem>IKO4</chem> , <chem>INaO4</chem> , <chem>IO4Rb</chem> , <chem>IO4Tl</chem> , <chem>LaMo4Na5O16</chem> , <chem>LaNbO4</chem> , <chem>LiSi</chem> , <chem>LuO4P</chem> , <chem>MoO4Pb</chem> , <chem>MoO4Sr</chem> , <chem>Mo4Na4O16U</chem> , <chem>Mo4Na4O16Zr</chem> , <chem>Na2O5Si2</chem> , <chem>Na5O16W4Y</chem> , <chem>NbO2</chem> , <chem>O24Re4Sr11</chem> , <chem>O2Ta</chem> , <chem>O4PbPd2</chem> , <chem>O4PbW</chem> , <chem>O4SiTi</chem> , <chem>O4SiZr</chem> , <chem>O4SrW</chem> , <chem>P4S12U</chem> , <chem>Pd2S4U</chem> ,
91	<chem>Ag3O4Sb</chem> , <chem>CBTh</chem> , <chem>LiNbO4Zn</chem> , <chem>Li2O4Te</chem> , <chem>O4TiZn2</chem> ,
92	<chem>AlKO2</chem> , <chem>AlliO2</chem> , <chem>As2O5</chem> , <chem>As4Mg</chem> , <chem>Au5F21Pr2</chem> , <chem>CO2</chem> , <chem>Ca</chem> , <chem>Ca2P4Si2</chem> , <chem>CdP2</chem> , <chem>F2Sn</chem> , <chem>GeO2</chem> , <chem>Ge2Lu2O7</chem> , <chem>Ge4Zr5</chem> , <chem>Hf5Si4</chem> , <chem>I8Pt3</chem> , <chem>La5Si4</chem> , <chem>O2Si</chem> , <chem>O2Te</chem> , <chem>P2Zn</chem> , <chem>P4Zn</chem> , <chem>S2Tl2</chem> , <chem>Si4Zr5</chem> ,
94	<chem>F6Li2Mo</chem> ,
96	<chem>Ag2HgO2</chem> , <chem>AuF22Sb4Xe4</chem> , <chem>B6Be</chem> , <chem>Ba3Sn2</chem> , <chem>CdP2</chem> , <chem>Ge</chem> , <chem>Na2O3Zn2</chem> , <chem>O2Te</chem> , <chem>P2Zn</chem> ,
97	<chem>Ca2O20Si8Th</chem> ,
98	<chem>As2Cd</chem> , <chem>O2Si</chem> ,
99	<chem>BaO3Ti</chem> , <chem>Bi2O6TiZn</chem> , <chem>Br3CsPb</chem> , <chem>Cl3CsPb</chem> , <chem>HfO3Sr</chem> , <chem>O3PbTi</chem> , <chem>O3SrZr</chem> ,
100	<chem>Ba2NaNb5O15</chem> , <chem>Ba2O8Si2Ti</chem> , <chem>K2Nb2O14Si4</chem> , <chem>La3N11Si6</chem> , <chem>O8Si2Sr2Ti</chem> ,
102	<chem>Al2Y3</chem> , <chem>Ca3Cd2</chem> , <chem>Cs2Hg6S7</chem> , <chem>K2O7Zn6</chem> , <chem>N2S4</chem> ,
104	<chem>HgI6Tl4</chem> ,
105	<chem>AlPS4</chem> , <chem>As2BaGe2</chem> , <chem>BaGe2P2</chem> ,
107	<chem>BaGe3Pt</chem> , <chem>BaPdSi3</chem> , <chem>BaPdSn3</chem> , <chem>BaPtSi3</chem> , <chem>BaPtSn3</chem> , <chem>Br8S9Ta4</chem> , <chem>CBaSi</chem> , <chem>CaPtSi3</chem> , <chem>Ca2Sb</chem> , <chem>Ge3PdSr</chem> , <chem>Ge3PtSr</chem> , <chem>Na6O5Pb</chem> , <chem>P2U</chem> , <chem>PdSn3Sr</chem> ,
108	<chem>Al3F19Pb5</chem> , <chem>ClF4NO</chem> , <chem>K2SnTe5</chem> , <chem>Rb2SnTe5</chem> , <chem>Si3Sr5</chem> ,
109	<chem>AlGeLa</chem> , <chem>AsNb</chem> , <chem>AsTa</chem> , <chem>Ba2S3</chem> , <chem>Ga2S2Te</chem> , <chem>Ga2Se2Te</chem> , <chem>Li8N2Se</chem> , <chem>Li8N2Te</chem> , <chem>NbP</chem> , <chem>PTa</chem> ,
110	<chem>As2Zn3</chem> ,
111	<chem>AgIn5Se8</chem> , <chem>AgIn5Te8</chem> , <chem>Ag2HgI4</chem> , <chem>As4Ge3</chem> , <chem>As4Si3</chem> , <chem>As4Sn3</chem> , <chem>C11N4</chem> , <chem>C3As4</chem> , <chem>C3N4</chem> , <chem>CdIn2Se4</chem> , <chem>F6KSB</chem> , <chem>Ga2S4Zn</chem> ,
112	<chem>AlPS4</chem> ,
113	<chem>AgTe2Y</chem> , <chem>B2Ca2O7Si</chem> , <chem>BaS3</chem> , <chem>BaSe3</chem> , <chem>BaTe3</chem> , <chem>Ba2Ge2MgO7</chem> , <chem>Ba2Ge2OS6Zn</chem> , <chem>Ba2Ge2O7Zn</chem> , <chem>Ba2MgO7Si2</chem> , <chem>BeCa2O7Si2</chem> , <chem>Be2F7LiNa2</chem> , <chem>Be2GeLa2O7</chem> , <chem>Be2GeO7Y2</chem> , <chem>Be2O7SiY2</chem> , <chem>Br3NbO</chem> , <chem>CN2</chem> , <chem>Ca2MgO7Si2</chem> , <chem>Ca2O7Si2Zn</chem> , <chem>CdMoO6Te</chem> , <chem>Cl3NbO</chem> , <chem>Cl6IP</chem> , <chem>Cs2O16S3U2</chem> ,

Part 13 of all the predicted materials with band crossings from **Cases 1 or 2:**

113	GaNb <sub>4</sub> S <sub>8</sub> , Ga <sub>2</sub> La <sub>2</sub> OS <sub>6</sub> Zn, LiNbO <sub>6</sub> W, Li <sub>6</sub> O <sub>7</sub> Si <sub>2</sub> , MgO <sub>7</sub> Si <sub>2</sub> Sr <sub>2</sub> , Mo <sub>3</sub> O <sub>12</sub> Y <sub>2</sub> , N <sub>4</sub> O <sub>3</sub> Si <sub>3</sub> Y <sub>2</sub> , O <sub>3</sub> W, O <sub>7</sub> Si <sub>2</sub> Sr <sub>2</sub> Zn,
114	Ba <sub>4</sub> Ga <sub>4</sub> Se <sub>12</sub> Sn, Ba <sub>4</sub> Ga <sub>5</sub> LiSe <sub>12</sub> , Bi <sub>2</sub> O <sub>3</sub> , C <sub>19</sub> Sc <sub>15</sub> , C <sub>19</sub> Y <sub>15</sub> , C <sub>32</sub> In <sub>4</sub> O <sub>32</sub> Re <sub>8</sub> , Ga <sub>4</sub> GePb <sub>4</sub> Se <sub>12</sub> , INb <sub>3</sub> Se <sub>12</sub> , Na <sub>3</sub> PS <sub>4</sub> , Na <sub>4</sub> S <sub>4</sub> Sn, Na <sub>4</sub> Se <sub>4</sub> Sn, O <sub>12</sub> Se <sub>4</sub> , O <sub>5</sub> SSn <sub>2</sub> , Pd <sub>4</sub> S, Pd <sub>4</sub> Se,
115	Bi <sub>2</sub> O <sub>3</sub> , Cl <sub>2</sub> Mg, Cs <sub>3</sub> Li <sub>2</sub> , F <sub>2</sub> OPb <sub>2</sub> , GaHf <sub>2</sub> Sb <sub>3</sub> , Li <sub>3</sub> N <sub>2</sub> Na <sub>3</sub> ,
116	BiF <sub>6</sub> K, F <sub>6</sub> KNb, F <sub>6</sub> Pb <sub>2</sub> , Ge <sub>7</sub> Re <sub>4</sub> , O <sub>2</sub> Si,
117	AuBi <sub>2</sub> NaO <sub>5</sub> , Ca <sub>2</sub> Ge <sub>7</sub> O <sub>16</sub> , Cd <sub>2</sub> Ge <sub>7</sub> O <sub>16</sub> , O <sub>4</sub> Pb <sub>3</sub> , PdRb <sub>2</sub> Se <sub>16</sub> ,
118	B, CB <sub>24</sub> Mg <sub>2</sub> , O <sub>2</sub> Si, O <sub>6</sub> Sb <sub>2</sub> Zn, P <sub>2</sub> S <sub>8</sub> Zn <sub>3</sub> ,
120	AgAsF <sub>10</sub> Xe <sub>2</sub> , AgMgSb, AlCsF <sub>4</sub> , AlF <sub>4</sub> Rb, Br <sub>13</sub> Cd <sub>3</sub> Cs <sub>7</sub> , O <sub>2</sub> Si, O <sub>6</sub> P <sub>4</sub> S <sub>4</sub> ,
121	AgClO <sub>4</sub> , Ag <sub>2</sub> BaGeS <sub>4</sub> , Ag <sub>2</sub> CdI <sub>4</sub> , Ag <sub>2</sub> KPS <sub>4</sub> , Ag <sub>2</sub> KS <sub>4</sub> SB, Ag <sub>2</sub> S <sub>4</sub> SnZn, AsHgS <sub>3</sub> Tl, As <sub>22</sub> Ba <sub>13</sub> Si <sub>6</sub> Sn <sub>8</sub> , AuPb <sub>3</sub> , CK <sub>4</sub> O <sub>4</sub> , CLi <sub>4</sub> O <sub>4</sub> , CNa <sub>4</sub> O <sub>4</sub> , CaGeLi <sub>2</sub> O <sub>4</sub> , CaLi <sub>2</sub> O <sub>4</sub> Si, CdGeTe <sub>4</sub> Tl <sub>2</sub> , CdIn <sub>2</sub> Se <sub>4</sub> , CdK <sub>2</sub> Se <sub>4</sub> Sn, CdSnTe <sub>4</sub> Tl <sub>2</sub> , ClCsF <sub>3</sub> Sb, F <sub>9</sub> NaTh <sub>2</sub> , GeHgTe <sub>4</sub> Tl <sub>2</sub> , GeLi <sub>2</sub> PbS <sub>4</sub> , GeO <sub>8</sub> Zr <sub>3</sub> , HgK <sub>2</sub> Se <sub>4</sub> Sn, HgRb <sub>2</sub> SnTe <sub>4</sub> , HgSe <sub>4</sub> SiTl <sub>2</sub> , HgSnTe <sub>4</sub> Tl <sub>2</sub> , Mo <sub>3</sub> P, NbO <sub>8</sub> Rb <sub>3</sub> , O <sub>2</sub> Si, O <sub>8</sub> Rb <sub>3</sub> Ta,
122	AgAlS <sub>2</sub> , AgAlSe <sub>2</sub> , AgAlTe <sub>2</sub> , AgGaS <sub>2</sub> , AgGaSe <sub>2</sub> , AgGaTe <sub>2</sub> , AgInS <sub>2</sub> , AgInSe <sub>2</sub> , AgInTe <sub>2</sub> , AlLiTe <sub>2</sub> , As <sub>2</sub> BeSi, As <sub>2</sub> CdGe, As <sub>2</sub> CdSi, As <sub>2</sub> CdSn, As <sub>2</sub> GeMg, As <sub>2</sub> GeZn, As <sub>2</sub> MgSi, As <sub>2</sub> SiZn, As <sub>2</sub> SnZn, As <sub>3</sub> Mg <sub>4</sub> NaO <sub>12</sub> , BLiO <sub>2</sub> , B <sub>2</sub> O <sub>4</sub> Pd, B <sub>6</sub> CsLiO <sub>10</sub> , BeN <sub>2</sub> Si, BeP <sub>2</sub> Si, BeSb <sub>2</sub> Si, CBeN <sub>2</sub> , CKN <sub>3</sub> O <sub>6</sub> , CMgN <sub>2</sub> , CN <sub>2</sub> , CN <sub>2</sub> Zn, CO <sub>2</sub> , C <sub>2</sub> HgN <sub>2</sub> , C <sub>3</sub> N <sub>3</sub> P, CaGeN <sub>2</sub> , CdGeP <sub>2</sub> , CdP <sub>2</sub> Si, CdP <sub>2</sub> Sn, CdSb <sub>2</sub> Sn, CdTe <sub>2</sub> Zn, Cl <sub>10</sub> N <sub>2</sub> S <sub>2</sub> Sb <sub>2</sub> , Cl <sub>2</sub> Zn, F <sub>4</sub> OU, F <sub>5</sub> U, GaLiO <sub>6</sub> Se <sub>2</sub> , GaLiTe <sub>2</sub> , GeMgP <sub>2</sub> , GeP <sub>2</sub> Zn, GeS <sub>2</sub> , GeSe <sub>2</sub> , HgP <sub>2</sub> Si, I <sub>2</sub> P <sub>4</sub> Se <sub>3</sub> , InLiSe <sub>2</sub> , InLiTe <sub>2</sub> , LiN <sub>2</sub> P, MgN <sub>2</sub> Si, MgP <sub>2</sub> Si, MgSb <sub>2</sub> Si, N <sub>2</sub> NaP, Na <sub>2</sub> S <sub>4</sub> , Na <sub>2</sub> Se <sub>4</sub> , O <sub>2</sub> Si, O <sub>4</sub> SiZn <sub>2</sub> , P <sub>2</sub> SiZn, S <sub>2</sub> Si, Sb <sub>18</sub> Zr <sub>11</sub> ,
123	AgPPd <sub>5</sub> , AgSbTe <sub>2</sub> , AlF <sub>4</sub> K, AlF <sub>4</sub> Na, AlF <sub>4</sub> Rb, AlF <sub>4</sub> Tl, AlF <sub>5</sub> K <sub>2</sub> , As <sub>2</sub> BaOTi <sub>2</sub> , As <sub>3</sub> Cd <sub>4</sub> Cs, As <sub>3</sub> CsZn <sub>4</sub> , As <sub>3</sub> RbZn <sub>4</sub> , BCa <sub>3</sub> N <sub>3</sub> , Ba, BaGe <sub>3</sub> Mg <sub>4</sub> , BaMg <sub>4</sub> Si <sub>3</sub> , BaOSb <sub>2</sub> Ti <sub>2</sub> , BaO <sub>3</sub> Ti, Ba <sub>3</sub> N <sub>2</sub> OZn, BiLi, BiNa, Bi <sub>2</sub> ClLuO <sub>4</sub> , Bi <sub>2</sub> ILaO <sub>4</sub> , Bi <sub>4</sub> ClO <sub>8</sub> Ta, Br <sub>4</sub> K <sub>2</sub> Pd, Br <sub>4</sub> K <sub>2</sub> Pt, CPd <sub>3</sub> Sn, C <sub>2</sub> AgK, C <sub>2</sub> AuNa, CaF <sub>2</sub> , Ca <sub>2</sub> O <sub>10</sub> RbTa <sub>3</sub> , CdHg <sub>2</sub> Ti, ClNa <sub>3</sub> , Cl <sub>4</sub> Cs <sub>2</sub> Pd, Cl <sub>4</sub> K <sub>2</sub> Pd, Cl <sub>4</sub> K <sub>2</sub> Pt, Cl <sub>4</sub> PdTl <sub>2</sub> , CsI, CsNb <sub>3</sub> O <sub>10</sub> Sr <sub>2</sub> , CsO <sub>10</sub> Sr <sub>2</sub> Ta <sub>3</sub> , HgTi, HgZr, LaO <sub>7</sub> RbTa <sub>2</sub> , Li <sub>5</sub> N <sub>2</sub> Na, MgPt <sub>3</sub> , MoPt <sub>3</sub> , N <sub>3</sub> Rb, NaNbO <sub>3</sub> , NaO <sub>3</sub> Ta, Nb <sub>3</sub> O <sub>10</sub> RbSr <sub>2</sub> , O <sub>3</sub> PbTi, P <sub>3</sub> RbZn <sub>4</sub> , Pb <sub>3</sub> Sr, Pd <sub>3</sub> Sn, Pt <sub>5</sub> SiSn,
124	Au <sub>2</sub> CdF <sub>8</sub> , Au <sub>2</sub> F <sub>8</sub> Hg, I <sub>3</sub> Nb <sub>10</sub> Se <sub>40</sub> ,
125	AgK <sub>3</sub> Se <sub>8</sub> Sn <sub>3</sub> , AgRb <sub>3</sub> Se <sub>8</sub> Sn <sub>3</sub> , Ag <sub>2</sub> BaHg <sub>2</sub> O <sub>4</sub> , Al <sub>2</sub> BaTe <sub>4</sub> , As <sub>4</sub> CaNa <sub>2</sub> O <sub>12</sub> , K <sub>3</sub> NaSe <sub>8</sub> Sn <sub>3</sub> , O <sub>2</sub> Si, Pb <sub>4</sub> Pt,
126	Al <sub>4</sub> Bi <sub>2</sub> S <sub>8</sub> , Al <sub>4</sub> Bi <sub>2</sub> Se <sub>8</sub> , Bi <sub>2</sub> Ga <sub>4</sub> S <sub>8</sub> , Bi <sub>2</sub> Ga <sub>4</sub> Se <sub>8</sub> , K <sub>8</sub> Tl <sub>10</sub> Zn, LaMo <sub>2</sub> O <sub>8</sub> Rb,
127	AlF <sub>3</sub> , AlF <sub>4</sub> K, AlF <sub>4</sub> Rb, AlPt <sub>3</sub> , AuBi <sub>5</sub> Na <sub>2</sub> O <sub>11</sub> , B <sub>4</sub> Ca, B <sub>4</sub> La, B <sub>4</sub> Lu, B <sub>4</sub> U, B <sub>4</sub> Y, BaCl <sub>2</sub> Hg <sub>2</sub> O <sub>2</sub> , BaLa <sub>2</sub> O <sub>5</sub> Pd, BaLa <sub>2</sub> O <sub>5</sub> Pt, BaO <sub>5</sub> PdY <sub>2</sub> , Ba <sub>3</sub> F <sub>12</sub> In <sub>2</sub> , Ba <sub>4</sub> In <sub>2</sub> S <sub>5</sub> Te <sub>2</sub> , Ba <sub>4</sub> In <sub>2</sub> Se <sub>5</sub> Te <sub>2</sub> , CB <sub>2</sub> Lu, CaO <sub>3</sub> Si, Ca <sub>2</sub> Ge <sub>2</sub> Sn, CdGe <sub>2</sub> Y <sub>2</sub> , CsF <sub>5</sub> K <sub>2</sub> Pd, CsF <sub>7</sub> Rb <sub>2</sub> Si, CsI <sub>3</sub> Sn, Cs <sub>3</sub> F <sub>7</sub> Ge, Cs <sub>3</sub> F <sub>7</sub> Si, Cs <sub>3</sub> F <sub>7</sub> Ti, F <sub>3</sub> MgNa, F <sub>5</sub> K <sub>2</sub> PdRb, F <sub>5</sub> PdRb <sub>3</sub> , F <sub>7</sub> K <sub>3</sub> Si, F <sub>7</sub> Rb <sub>3</sub> Ti, GaPt <sub>3</sub> , GeTe <sub>5</sub> Tl <sub>2</sub> , HfO <sub>3</sub> Sr, Hf <sub>3</sub> In <sub>4</sub> , Hg <sub>2</sub> I <sub>2</sub> PbS <sub>2</sub> , In <sub>4</sub> Ti <sub>3</sub> , K <sub>2</sub> LaNb <sub>5</sub> O <sub>15</sub> , K <sub>2</sub> LaO <sub>15</sub> Ta <sub>5</sub> , K <sub>3</sub> Li <sub>2</sub> Nb <sub>5</sub> O <sub>15</sub> , Li <sub>2</sub> Sn <sub>5</sub> , NaO <sub>3</sub> Ta, O <sub>3</sub> SrZr, Pb <sub>3</sub> Sr <sub>2</sub> , Pt <sub>3</sub> Si, Si <sub>2</sub> Th <sub>3</sub> , Si <sub>2</sub> U <sub>3</sub> ,

Part 14 of all the predicted materials with band crossings from **Cases 1 or 2**:

128	<chem>Al3F14Na5</chem> , <chem>Br4STl6</chem> , <chem>Br6HgTl4</chem> , <chem>Br6In2Zr</chem> , <chem>Br6K2Te</chem> , <chem>Br6Rb2U</chem> , <chem>Br6TeTl2</chem> , <chem>CdI6In4</chem> , <chem>CdI6Tl4</chem> , <chem>Cl4STl6</chem> , <chem>Cl6K2Sn</chem> , <chem>F14In3K5</chem> , <chem>F6HfK2</chem> , <chem>HgI6Tl4</chem> , <chem>INb3Se12</chem> , <chem>I4STl6</chem> , <chem>I4SeTl6</chem> , <chem>I6K2Pt</chem> , <chem>I6Rb2Te</chem> ,
129	<chem>AcBrO</chem> , <chem>AcClO</chem> , <chem>AgAsOTh</chem> , <chem>AgBaFS</chem> , <chem>AgBaFSe</chem> , <chem>AgBaFTe</chem> , <chem>AgBrOPb</chem> , <chem>AgBr2Cs</chem> , <chem>AgCl2Cs</chem> , <chem>AgFSSr</chem> , <chem>AgFSeSr</chem> , <chem>AgFSrTe</chem> , <chem>AgKSe</chem> , <chem>AgLaOS</chem> , <chem>AgLaO4Ti</chem> , <chem>AgLaSb2</chem> , <chem>AgOPTh</chem> , <chem>AgSb2Y</chem> , <chem>AlBaFGe</chem> , <chem>AlF3</chem> , <chem>AlGeNa</chem> , <chem>AlNaSi</chem> , <chem>Al2Au2Sr</chem> , <chem>Al2Au2Th</chem> , <chem>AsBaFZn</chem> , <chem>AsBeLi</chem> , <chem>AsCaRb</chem> , <chem>AsCdK</chem> , <chem>AsFSrZn</chem> , <chem>AsGeNb</chem> , <chem>AsKMg</chem> , <chem>AsLaOZn</chem> , <chem>AsMgNa</chem> , <chem>AsNaZn</chem> , <chem>AsPU</chem> , <chem>As2PdU</chem> , <chem>As2U</chem> , <chem>AuLaSb2</chem> , <chem>Au2Ga2Sr</chem> , <chem>Au2Sn2Sr</chem> , <chem>BaF4Sn</chem> , <chem>BaGeMg</chem> , <chem>BaHfN2</chem> , <chem>BaMgPb</chem> , <chem>BaMgSn</chem> , <chem>BaMg2Pb2</chem> , <chem>BaMg2Sn2</chem> , <chem>BaN2Zr</chem> , <chem>BaO</chem> , <chem>BaPd2Sb2</chem> , <chem>BaSn2Zn2</chem> , <chem>Ba2BrInO3</chem> , <chem>Ba2Br2F10Pb4</chem> , <chem>Ba2ClInO3</chem> , <chem>Ba2F10I2Pb4</chem> , <chem>Ba2FInO3</chem> , <chem>Ba2OTe</chem> , <chem>BeLiP</chem> , <chem>Be2CaGe2</chem> , <chem>BiBrO</chem> , <chem>BiCaK</chem> , <chem>BiClO</chem> , <chem>BiFO</chem> , <chem>BiIO</chem> , <chem>BiIO3Te</chem> , <chem>BiLaOS2</chem> , <chem>BiLaOSe2</chem> , <chem>BiLiO4Pd2</chem> , <chem>Bi2LaLi</chem> , <chem>Bi2OS2</chem> , <chem>Bi2Pd2Sr</chem> , <chem>BrFPb</chem> , <chem>BrLaO</chem> , <chem>BrLuO</chem> , <chem>BrNU</chem> , <chem>Br2CsLi</chem> , <chem>CaClF</chem> , <chem>CaGaN</chem> , <chem>CaGa4</chem> , <chem>CaRbSb</chem> , <chem>CdHf</chem> , <chem>CdKSb</chem> , <chem>CdTl</chem> , <chem>CdZr</chem> , <chem>Cd3O5Si</chem> , <chem>ClFPb</chem> , <chem>ClLaO</chem> , <chem>ClLaTe</chem> , <chem>CINTh</chem> , <chem>CINU</chem> , <chem>ClOY</chem> , <chem>Cl2CsLi</chem> , <chem>CsF4Ti</chem> , <chem>CsNaS</chem> , <chem>CsNaSe</chem> , <chem>CsNaTe</chem> , <chem>FIPb</chem> , <chem>FLaO</chem> , <chem>FLaS</chem> , <chem>FOY</chem> , <chem>FTl</chem> , <chem>F4KMoNaO2</chem> , <chem>F4KNaO2W</chem> , <chem>F4PbSn</chem> , <chem>F5KNaNbO</chem> , <chem>GeHfS</chem> , <chem>GeHfSe</chem> , <chem>GeHfTe</chem> , <chem>GeLi2O5Ti</chem> , <chem>GeNa2O5Ti</chem> , <chem>GeNbSb</chem> , <chem>GeSU</chem> , <chem>GeSzr</chem> , <chem>GeSeZr</chem> , <chem>Ge2Pt2Th</chem> , <chem>Ge2Pt2U</chem> , <chem>HfSSI</chem> , <chem>HfSb2</chem> , <chem>HfSeSi</chem> , <chem>HfSiTe</chem> , <chem>ILaO</chem> , <chem>ILuO</chem> , <chem>INTh</chem> , <chem>INU</chem> , <chem>In9Li2Y5</chem> , <chem>KLaNaNbO5</chem> , <chem>KLaNaO5Ta</chem> , <chem>KLaO4Ti</chem> , <chem>KLiS</chem> , <chem>KLiSe</chem> , <chem>KLiTe</chem> , <chem>KMgP</chem> , <chem>KMgSb</chem> , <chem>KNaO</chem> , <chem>LaLiO4Ti</chem> , <chem>LaN</chem> , <chem>LaNaO4Ti</chem> , <chem>LaOPZn</chem> , <chem>LaOSbZn</chem> , <chem>LaSbTe</chem> , <chem>LiNaS</chem> , <chem>LiRbS</chem> , <chem>LiRbSe</chem> , <chem>Li2N2Na4</chem> , <chem>Li2O5SiTi</chem> , <chem>MgNaSb</chem> , <chem>N2SrTi</chem> , <chem>NaORb</chem> , <chem>NaPZn</chem> , <chem>NaRbS</chem> , <chem>NaSbZn</chem> , <chem>Na2O5SiTi</chem> , <chem>OPb</chem> , <chem>OSTh</chem> , <chem>OSU</chem> , <chem>OSeTh</chem> , <chem>OSeU</chem> , <chem>OSiZr</chem> , <chem>OSn</chem> , <chem>OTeTh</chem> , <chem>OTeU</chem> , <chem>O3W</chem> , <chem>P2U</chem> , <chem>PdSb2U</chem> , <chem>Pd2Sb2Sr</chem> , <chem>Pt2Si2Th</chem> , <chem>SSiU</chem> , <chem>SSiZr</chem> , <chem>SZr</chem> , <chem>Sb2U</chem> , <chem>Sc</chem> , <chem>SeSiZr</chem> , <chem>SeTa2</chem> , <chem>SeTi</chem> , <chem>SeZn</chem> , <chem>SiTeZr</chem> , <chem>SnTeU</chem> , <chem>SnTeZr</chem> ,
130	<chem>Ba5Ge3</chem> , <chem>Ba5Si3</chem> , <chem>Bi2O4Pd</chem> , <chem>Ca5Ge3</chem> , <chem>ClSe2Tl5</chem> , <chem>Cl4Na2Pd</chem> , <chem>Ga3Y5</chem> , <chem>IK3O5</chem> , <chem>O3W</chem> , <chem>O5SiSr3</chem> , <chem>PbSe3Tl4</chem> , <chem>S3SnTl4</chem> ,
131	<chem>C2Th</chem> , <chem>CaO4Pt2</chem> , <chem>F6PbSr</chem> , <chem>IPdTe</chem> , <chem>LiNSr</chem> ,
132	<chem>AgF6Ta</chem> , <chem>Ag2Cs2S4Ti</chem> ,
133	<chem>PTa3</chem> ,
135	<chem>CB2Lu</chem> , <chem>CB2Sc</chem> , <chem>Cs</chem> , <chem>O2Se</chem> , <chem>O4Pb3</chem> , <chem>O4Sb2Zn</chem> , <chem>PdSe</chem> ,
136	<chem>Ag5CsSe3</chem> , <chem>Ag5CsTe3</chem> , <chem>Al2Hf3</chem> , <chem>Al2Lu3</chem> , <chem>Al2Y3</chem> , <chem>Al2Zr3</chem> , <chem>As2BrLa3O7</chem> , <chem>AuLi3O3</chem> , <chem>AuNa3O2</chem> , <chem>BLi3N2</chem> , <chem>BN</chem> , <chem>BaCd4Pt2</chem> , <chem>BaHg2Tl2</chem> , <chem>BaHg2Tl2</chem> , <chem>BaIn2La2O7</chem> , <chem>BaLa2O7Sc2</chem> , <chem>Ba3Ge4</chem> , <chem>Ba3S7Zr2</chem> , <chem>Ba3Si4</chem> , <chem>BeO</chem> , <chem>Be2K2Na4O5</chem> , <chem>BiLi3O4</chem> , <chem>Br2Ca</chem> , <chem>CO2</chem> , <chem>C2Mg</chem> , <chem>Ca10Mg2Sb9</chem> , <chem>CaCl2</chem> , <chem>Cd4Pt2Sr</chem> , <chem>Cl3NbO</chem> , <chem>Cl3OW</chem> , <chem>Cs2K2O5Te</chem> , <chem>F2Kr</chem> , <chem>F2Mg</chem> , <chem>F2Pd</chem> , <chem>F2Zn</chem> , <chem>F6GeLi2</chem> , <chem>F6Li2Mo</chem> , <chem>F6Li2Pd</chem> , <chem>F6Li2Pt</chem> , <chem>F6Na2Sn</chem> , <chem>Ga2O6Te</chem> , <chem>Ga3Re</chem> , <chem>Ga5Nb4</chem> , <chem>GeO2</chem> , <chem>Hg2Na3</chem> , <chem>I3OW</chem> , <chem>KPPdS4</chem> , <chem>LiO3RbZn2</chem> , <chem>Li2Sr3</chem> , <chem>MgO6Sb2</chem> , <chem>MgO6Ta2</chem> , <chem>MoO2</chem> , <chem>N2</chem> , <chem>O2Si</chem> , <chem>O2Sn</chem> , <chem>O2Ti</chem> , <chem>O2W</chem> , <chem>O6Sb2Zn</chem> ,

Part 15 of all the predicted materials with band crossings from **Cases 1 or 2:**

137	<chem>As2Zn3</chem> , <chem>BLiSi2</chem> , <chem>B4Cl4</chem> , <chem>Ba2LiN</chem> , <chem>Ba2S6Th</chem> , <chem>Ba2S6U</chem> , <chem>CaO3Si</chem> , <chem>Cd4F6O</chem> , <chem>Cl2Zn</chem> , <chem>F2OPb2</chem> , <chem>GeS2</chem> , <chem>HfO2</chem> , <chem>HgI2</chem> , <chem>Hg2I4</chem> , <chem>Li10O9Zn4</chem> , <chem>Li6MoN4</chem> , <chem>Li6N4W</chem> , <chem>Li6O4Zn</chem> , <chem>O2Zr</chem> , <chem>P2Zn3</chem> ,
138	<chem>AuBr</chem> , <chem>CLiO2</chem> , <chem>Cl2</chem> , <chem>Cl6Se4Zr</chem> , <chem>F6Pb2Zn</chem> , <chem>O4SnSr2</chem> ,
139	<chem>AgBrO3</chem> , <chem>AgClO3</chem> , <chem>AgCsO</chem> , <chem>AgNaO</chem> , <chem>AgORb</chem> , <chem>Ag2BaGe2</chem> , <chem>Ag2BaSn2</chem> , <chem>Ag2Cl6Cs2</chem> , <chem>Ag2La2O10Ti3</chem> , <chem>Al2BaGe2</chem> , <chem>Al2CaGa2</chem> , <chem>Al2FK4Nb11O20</chem> , <chem>Al2Pd5U</chem> , <chem>Al3Hf</chem> , <chem>AsCa2</chem> , <chem>AsTiZr</chem> , <chem>As2BaZn2</chem> , <chem>As2Ba2O2Zn3</chem> , <chem>As2Ca4O</chem> , <chem>AuC-sO</chem> , <chem>Au2Be</chem> , <chem>Au2Br6Cs2</chem> , <chem>Au2CaGe2</chem> , <chem>Au2CaSi2</chem> , <chem>Au2Cl6Cs2</chem> , <chem>Au2Cs2I6</chem> , <chem>Au2Ge2Sr</chem> , <chem>Au2Si2Sr</chem> , <chem>Au2Si2U</chem> , <chem>Ba11Bi10</chem> , <chem>BaBi2Cd</chem> , <chem>BaBi2Zn</chem> , <chem>BaBi4I2O4</chem> , <chem>BaCdSb2</chem> , <chem>BaCd2Ge2</chem> , <chem>BaGe2Mg2</chem> , <chem>BaMg2Si2</chem> , <chem>BaP2Zn2</chem> , <chem>BaP4Pd2</chem> , <chem>BaSi2</chem> , <chem>BaSi2Zn2</chem> , <chem>Ba2F2O2Pd</chem> , <chem>Ba2F6Zn</chem> , <chem>Ba2N2Zn</chem> , <chem>Ba2O4Pb</chem> , <chem>Ba2O4Sn</chem> , <chem>Ba2O4Zr</chem> , <chem>Ba3Br2In2O5</chem> , <chem>Ba3Cl2In2O5</chem> , <chem>Ba3Cl2O5Tl2</chem> , <chem>Ba3S7Zr2</chem> , <chem>Ba4OSb2</chem> , <chem>Be12Mo</chem> , <chem>Be12W</chem> , <chem>BePd2</chem> , <chem>Bi10Ca11</chem> , <chem>Bi10Sr11</chem> , <chem>BiCa2</chem> , <chem>Bi2Ca4O</chem> , <chem>Bi2CdSr</chem> , <chem>Bi2O2Se</chem> , <chem>Bi2O9SrTa2</chem> , <chem>Bi2Pd</chem> , <chem>Bi2SrZn</chem> , <chem>Br2Ca3Si</chem> , <chem>Br2Hg2</chem> , <chem>Br3Li7O2</chem> , <chem>C</chem> , <chem>CLi2N2</chem> , <chem>C2PtU2</chem> , <chem>C2Si2U3</chem> , <chem>C4AuBa4KO4</chem> , <chem>CaCs2F4</chem> , <chem>CaGe2Zn2</chem> , <chem>CaIn</chem> , <chem>CaO3Si</chem> , <chem>CaSi2Zn2</chem> , <chem>CaSi3</chem> , <chem>Ca2GeO4</chem> , <chem>Ca2N2Zn</chem> , <chem>Ca2O4Si</chem> , <chem>Ca2Pd3Sb4</chem> , <chem>Ca4OP2</chem> , <chem>Ca4OSb2</chem> , <chem>CdCl4Rb2</chem> , <chem>CdHf2</chem> , <chem>CdHg2</chem> , <chem>Cd2Ga2Sr</chem> , <chem>Cd2Ge2Sr</chem> , <chem>Cd2Hg</chem> , <chem>Cl10K4ORe2</chem> , <chem>Cl2Hg2</chem> , <chem>Cl4K2Mg</chem> , <chem>Cl6Cs2HgPd</chem> , <chem>Cl7Cs3Mg2</chem> , <chem>CsF3Li2</chem> , <chem>Cs2F4Hg</chem> , <chem>Cs2HgO2</chem> , <chem>Cs2I6Pd</chem> , <chem>Cs3F6Tl</chem> , <chem>Cs3F6Y</chem> , <chem>F2Hg2</chem> , <chem>F2Xe</chem> , <chem>F3La</chem> , <chem>F4HgRb2</chem> , <chem>F4K2Mg</chem> , <chem>F4MgRb2</chem> , <chem>F4Pb</chem> , <chem>F4Sn</chem> , <chem>F6Rb3Tl</chem> , <chem>F6Rb3Y</chem> , <chem>F7K3Zn2</chem> , <chem>F8Na2U</chem> , <chem>F8Na3Pa</chem> , <chem>Ga10Hf11</chem> , <chem>Ga3K2</chem> , <chem>Ga3Zr</chem> , <chem>Ga4Ti2Zr</chem> , <chem>GeLaSc</chem> , <chem>GeSTh</chem> , <chem>GeSeU</chem> , <chem>GeTeU</chem> , <chem>Ge2Pd2Th</chem> , <chem>Ge2Pt2Th</chem> , <chem>Ge2Pt2U</chem> , <chem>Ge2SrZn2</chem> , <chem>Ge4In6La11</chem> , <chem>Hf2Zn</chem> , <chem>Hg</chem> , <chem>Hg2I2</chem> , <chem>Hg2In2Sr</chem> , <chem>Hg2Mg</chem> , <chem>In3Rb2</chem> , <chem>In3Zr</chem> , <chem>K2Mg5Sn3</chem> , <chem>K2O4U</chem> , <chem>K2O7SrTa2</chem> , <chem>La11Sn10</chem> , <chem>LaSbSc</chem> , <chem>LaScSi</chem> , <chem>La2O4Pd</chem> , <chem>LiPd2Tl</chem> , <chem>Li2O7SrTa2</chem> , <chem>LuSbZr</chem> , <chem>MgO6ReSr2</chem> , <chem>MgPd3</chem> , <chem>Mg2O4Si</chem> , <chem>Mo3Sb7</chem> , <chem>N2Sr2Zn</chem> , <chem>N2TeTh2</chem> , <chem>OP2Sr4</chem> , <chem>O2TeU2</chem> , <chem>O4Rb2U</chem> , <chem>O4SnSr2</chem> , <chem>O4Sr2Ti</chem> , <chem>O7Sr3Ti2</chem> , <chem>PTeU</chem> , <chem>PdTi2</chem> , <chem>Pd2Si2Th</chem> , <chem>Pd2Ti</chem> , <chem>Pt2Si2Th</chem> , <chem>Pt2Si2U</chem> , <chem>Pt2Th</chem> , <chem>Pt8Ti</chem> , <chem>SSiT</chem> , <chem>SbYZr</chem> , <chem>SeSiTh</chem> , <chem>SeSiU</chem> , <chem>Si</chem> , <chem>Sn</chem> , <chem>ThZn4</chem> , <chem>Ti2Zn</chem> ,
140	<chem>AgAuF4</chem> , <chem>AgF4K</chem> , <chem>AgF4Na</chem> , <chem>AgI2Tl</chem> , <chem>AgN3</chem> , <chem>AlFO4Sr3</chem> , <chem>AlF4Tl</chem> , <chem>AlKTe2</chem> , <chem>AlLaO3</chem> , <chem>AlNaSe2</chem> , <chem>AlNaTe2</chem> , <chem>AlSe2Tl</chem> , <chem>AuF11Th2</chem> , <chem>AuF4K</chem> , <chem>AuF4Na</chem> , <chem>AuF4Rb</chem> , <chem>B2Mo5Si</chem> , <chem>BaBe2N2</chem> , <chem>BaF4Pd</chem> , <chem>BaLa2O5Zn</chem> , <chem>BaLa2S5Zn</chem> , <chem>BaO3Pb</chem> , <chem>BaO3Zr</chem> , <chem>BaTe2</chem> , <chem>BaTe5U2</chem> , <chem>Ba3ClInS4</chem> , <chem>Ba3ClInSe4</chem> , <chem>Ba3O5Si</chem> , <chem>Ba3S5Ti</chem> , <chem>Ba4Bi3KO</chem> , <chem>Ba4KOSb3</chem> , <chem>Ba4ORbSb3</chem> , <chem>Ba6S14Zn6Zr</chem> , <chem>BeTa2</chem> , <chem>Be4Ca2N4</chem> , <chem>Be4N4Sr2</chem> , <chem>Bi</chem> , <chem>Bi3In5</chem> , <chem>Br13Cd3Cs7</chem> , <chem>BrF4K</chem> , <chem>BrF4Rb</chem> , <chem>BrSe2Tl5</chem> , <chem>BrTe2Tl5</chem> , <chem>Br5CdCs3</chem> , <chem>Br5CsSn2</chem> , <chem>Br5Cs3Zn</chem> , <chem>Br5InSn2</chem> , <chem>Br5Pb2Rb</chem> , <chem>Br5RbSn2</chem> , <chem>Br5Sn2Tl</chem> , <chem>C2B2Ca</chem> , <chem>CaF4Pd</chem> , <chem>CaO3Si</chem> , <chem>CaO3Ti</chem> , <chem>Ca5Hg3</chem> , <chem>Cd3Sr5</chem> , <chem>Cl3Li5O</chem> , <chem>Cl5CsPb2</chem> , <chem>Cl5CsSn2</chem> , <chem>Cl5Cs3Zn</chem> , <chem>Cl5KSn2</chem> , <chem>FGaO4Sr3</chem> , <chem>F4PbPd</chem> , <chem>F4PdSr</chem> , <chem>GaInSe2</chem> , <chem>GaNaTe2</chem> , <chem>GaTe2Tl</chem> , <chem>Ga2Lu3</chem> , <chem>Ga2Sc3</chem> , <chem>Ga2Y3</chem> , <chem>Ga3Ta5</chem> , <chem>GeNb3</chem> , <chem>GePt3</chem> , <chem>Ge3Sr5</chem> , <chem>HfO3Sr</chem> , <chem>Hf2Si</chem> , <chem>ISe2Tl5</chem> , <chem>I5InPb2</chem> , <chem>I5InSn2</chem> , <chem>I5InSr2</chem> , <chem>I5KSn2</chem> , <chem>InKTe2</chem> , <chem>InNaTe2</chem> , <chem>InRbTe2</chem> , <chem>InS2Tl</chem> , <chem>InSe2Tl</chem> , <chem>InTe</chem> , <chem>InTe2Tl</chem> , <chem>In5Sb3</chem> , <chem>KN3</chem> , <chem>Lu7Sb3</chem> , <chem>Mg2Pt</chem> , <chem>MoO3Sr</chem> , <chem>NO2SrTa</chem> , <chem>N3Tl</chem> , <chem>NaPPdS4</chem> , <chem>O3SnSr</chem> , <chem>O3SrTi</chem> , <chem>O3SrZr</chem> , <chem>PbSe2</chem> , <chem>PbSe3Tl4</chem> , <chem>Pb2Pt</chem> , <chem>PtTl2</chem> , <chem>STl</chem> , <chem>S2Sr</chem> , <chem>S2Tl2</chem> , <chem>Sb</chem> , <chem>SbTi3</chem> , <chem>Sb2Ti</chem> , <chem>Sc</chem> , <chem>SeTl</chem> , <chem>Se2Tl2</chem> , <chem>Se3SnTl4</chem> , <chem>SiTa2</chem> , <chem>SiU3</chem> , <chem>SiZr2</chem> , <chem>Si3Sr5</chem> , <chem>SnTe3Tl4</chem> , <chem>SnTe5Tl2</chem> , <chem>Sn3Sr5</chem> ,
141	<chem>AgLi</chem> , <chem>Ag8O4S2Si</chem> , <chem>ALLi</chem> , <chem>Al2Mg</chem> , <chem>Al2S3</chem> , <chem>Al2Ti</chem> , <chem>AsLuO4</chem> , <chem>AsO4Sc</chem> , <chem>AsO4Y</chem> , <chem>As2Cs2O8Th</chem> , <chem>AuBr</chem> ,

Part 16 of all the predicted materials with band crossings from **Cases 1 or 2:**

141	AuCl, BF <sub>5</sub> Li <sub>2</sub> , BLi <sub>3</sub> N <sub>2</sub> , BMo, BNbO <sub>4</sub> , BO <sub>4</sub> Ta, BW, BaCd <sub>11</sub> , BaGe <sub>2</sub> , BaO <sub>7</sub> U <sub>2</sub> , BeF <sub>12</sub> Li <sub>6</sub> Zr, Br <sub>12</sub> Rb <sub>4</sub> Sb <sub>2</sub> , BrCsO <sub>4</sub> , Br <sub>4</sub> Th, Br <sub>6</sub> Cs <sub>2</sub> Sb, CaIn <sub>2</sub> O <sub>4</sub> , CaSi <sub>2</sub> , CaZn <sub>11</sub> , Cd <sub>11</sub> Sr, CdIn <sub>2</sub> O <sub>4</sub> , Cl <sub>2</sub> O, Cl <sub>6</sub> Cs <sub>2</sub> Sb, FMg <sub>2</sub> N, F <sub>2</sub> Na <sub>2</sub> O <sub>8</sub> SiU <sub>2</sub> , GaZr, Ga <sub>2</sub> Hf, Ga <sub>2</sub> Th, Ge, GeO <sub>4</sub> Th, HfO <sub>4</sub> Si, HgI <sub>2</sub> , I <sub>4</sub> Te, In <sub>2</sub> S <sub>3</sub> , In <sub>2</sub> Zr, LaO <sub>4</sub> P, LiO <sub>2</sub> Sc, Li <sub>4</sub> N <sub>2</sub> Sr, N <sub>2</sub> OSi <sub>2</sub> , NbP, O <sub>2</sub> Ti, O <sub>3</sub> U, O <sub>4</sub> SiTh, O <sub>4</sub> SiTi, PTa, PbU, S <sub>2</sub> Zr <sub>9</sub> , ScSn <sub>2</sub> , Si, Si <sub>2</sub> Sr, Si <sub>2</sub> Th, Si <sub>2</sub> U, Sn, SrZn <sub>11</sub> ,
142	Al <sub>2</sub> CaCl <sub>8</sub> , Al <sub>2</sub> Cl <sub>8</sub> Sr, As <sub>2</sub> Zn <sub>3</sub> , Au <sub>3</sub> Zn, BeI <sub>2</sub> , Be <sub>3</sub> P <sub>2</sub> , Br <sub>2</sub> Zn, C <sub>2</sub> Na <sub>2</sub> , CsGe, CsPb, CsSi, CsSn, Cs <sub>2</sub> PdSe <sub>8</sub> , Cs <sub>4</sub> Sn <sub>4</sub> , Ga <sub>2</sub> Pt, GeK, GeRb, KPb, KSi, KSn, K <sub>4</sub> Sn <sub>4</sub> , K <sub>8</sub> Pb <sub>8</sub> , LaPS <sub>4</sub> , NaP <sub>7</sub> , NaPb, NaSn, Na <sub>4</sub> Sn <sub>4</sub> , PbRb, Pb <sub>4</sub> Rb <sub>4</sub> , RbSi, RbSn, Rb <sub>4</sub> Sn <sub>4</sub> ,
143	Al <sub>5</sub> Mo, BaGe <sub>4</sub> O <sub>9</sub> , Ba <sub>3</sub> N <sub>4</sub> O <sub>9</sub> Si <sub>6</sub> , Br <sub>2</sub> Hg, C <sub>3</sub> N <sub>4</sub> , F <sub>6</sub> Na <sub>2</sub> U, Ge <sub>3</sub> O <sub>11</sub> Pb <sub>5</sub> , Ge <sub>9</sub> O <sub>33</sub> Pb <sub>15</sub> , K <sub>2</sub> O <sub>9</sub> Si <sub>3</sub> Zr, LaNb <sub>7</sub> O <sub>19</sub> , Li <sub>7</sub> O <sub>6</sub> Ta, MgO, Na <sub>4</sub> O <sub>12</sub> Ti <sub>5</sub> , S <sub>6</sub> ,
144	AsBBaO <sub>5</sub> , B <sub>2</sub> O <sub>3</sub> , Bi <sub>2</sub> O <sub>7</sub> Sn <sub>2</sub> , CsNO <sub>3</sub> , F <sub>4</sub> KTl, F <sub>4</sub> KY, Hg <sub>3</sub> O <sub>6</sub> S, TeZn,
145	BeCl <sub>2</sub> ,
146	Ag <sub>2</sub> Nb <sub>4</sub> O <sub>11</sub> , Ag <sub>3</sub> IS, AlLiO <sub>4</sub> Si, Al <sub>4</sub> B <sub>6</sub> O <sub>15</sub> , As <sub>12</sub> Sn <sub>3</sub> Si <sub>14</sub> , AsLiO <sub>4</sub> Zn, B <sub>2</sub> BaO <sub>4</sub> , B <sub>3</sub> Cl <sub>6</sub> N <sub>3</sub> , Ba <sub>3</sub> Lu <sub>4</sub> O <sub>9</sub> , Ba <sub>3</sub> O <sub>9</sub> Y <sub>4</sub> , Bi <sub>3</sub> Pds, C, CCs <sub>4</sub> O <sub>4</sub> , CK <sub>4</sub> O <sub>4</sub> , CNa <sub>4</sub> O <sub>4</sub> , CdPS <sub>3</sub> , Cl <sub>3</sub> CsGe, Cs <sub>6</sub> S <sub>27</sub> Ti <sub>6</sub> , F <sub>3</sub> MoNa <sub>3</sub> O <sub>3</sub> , GaLiO <sub>4</sub> Si, Ga <sub>4</sub> Pd <sub>7</sub> Zn <sub>3</sub> , GeLa <sub>2</sub> MgO <sub>6</sub> , IKO <sub>3</sub> , InMg <sub>3</sub> , KO <sub>12</sub> Sb <sub>3</sub> Zn <sub>4</sub> , K <sub>2</sub> O <sub>3</sub> Sn <sub>2</sub> , K <sub>2</sub> O <sub>9</sub> Si <sub>3</sub> Ti, K <sub>4</sub> O <sub>18</sub> Si <sub>6</sub> Sn <sub>2</sub> , Li <sub>2</sub> O <sub>6</sub> TeZr, Li <sub>7</sub> O <sub>6</sub> Sb, Mg <sub>9</sub> Sn <sub>5</sub> , Nb <sub>2</sub> O <sub>6</sub> Pb, O <sub>11</sub> PbTa <sub>4</sub> , Pd <sub>8</sub> Sb <sub>3</sub> , STl <sub>2</sub> ,
147	Al <sub>2</sub> BaO <sub>8</sub> Si <sub>2</sub> , As <sub>2</sub> K <sub>2</sub> S <sub>6</sub> Sn, As <sub>2</sub> S <sub>6</sub> SnTl <sub>2</sub> , As <sub>6</sub> BiK <sub>3</sub> Se <sub>12</sub> , Au <sub>7</sub> In <sub>3</sub> , BaCa <sub>2</sub> MgO <sub>8</sub> Si <sub>2</sub> , Ba <sub>3</sub> MgO <sub>8</sub> Si <sub>2</sub> , Bi <sub>2</sub> O <sub>6</sub> U, Bi <sub>2</sub> Pt, Br <sub>3</sub> InK, C <sub>3</sub> N <sub>4</sub> , Cd <sub>2</sub> Na <sub>14</sub> O <sub>9</sub> , Cd <sub>3</sub> Cl <sub>3</sub> P, F <sub>6</sub> KNaTh, Ge <sub>2</sub> K <sub>2</sub> O <sub>7</sub> Pb <sub>2</sub> , Ge <sub>9</sub> Pd <sub>25</sub> , InSiTe <sub>3</sub> , K <sub>2</sub> O <sub>3</sub> Te, K <sub>2</sub> O <sub>7</sub> Pb <sub>2</sub> Si <sub>2</sub> , K <sub>3</sub> Na <sub>8</sub> Se <sub>2</sub> , Li <sub>14</sub> N <sub>6</sub> O <sub>3</sub> P <sub>2</sub> , Li <sub>2</sub> N <sub>2</sub> Th, Li <sub>2</sub> N <sub>2</sub> U, Na <sub>2</sub> O <sub>3</sub> S, O <sub>7</sub> Si <sub>2</sub> Tl <sub>6</sub> , Os <sub>8</sub> U <sub>3</sub> , O <sub>9</sub> SZr <sub>3</sub> , Rb <sub>4</sub> Sb <sub>6</sub> Sn,
148	AgAsS <sub>2</sub> , AgBiP <sub>2</sub> Se <sub>6</sub> , AgI <sub>3</sub> Tl <sub>2</sub> , AgO <sub>3</sub> Sb, Ag <sub>2</sub> I <sub>6</sub> O <sub>18</sub> Ti, AlF <sub>3</sub> , AlF <sub>6</sub> K <sub>2</sub> Li, AlGeLiO <sub>4</sub> , AsCsF <sub>6</sub> , AsF <sub>6</sub> In, AsF <sub>6</sub> K, AsF <sub>6</sub> Li, AsF <sub>6</sub> Na, AsF <sub>6</sub> Rb, AsF <sub>6</sub> Tl, AsI <sub>3</sub> , AsLiO <sub>3</sub> , AuClO, AuF <sub>6</sub> Li, B <sub>2</sub> BaO <sub>6</sub> Ti, B <sub>2</sub> CaO <sub>6</sub> Sn, B <sub>2</sub> MgO <sub>6</sub> Sn, B <sub>6</sub> Ba <sub>2</sub> O <sub>12</sub> Pb, B <sub>6</sub> S <sub>12</sub> Si <sub>3</sub> , BaBiO <sub>3</sub> , BaF <sub>6</sub> Sn, Ba <sub>2</sub> BiLuO <sub>6</sub> , Ba <sub>2</sub> BiO <sub>6</sub> Sb, Ba <sub>2</sub> BiO <sub>6</sub> Ta, Ba <sub>2</sub> Bi <sub>2</sub> O <sub>6</sub> , Ba <sub>2</sub> LaO <sub>6</sub> Sb, Ba <sub>2</sub> LaO <sub>6</sub> Ta, Ba <sub>2</sub> O <sub>6</sub> SrTe, Ba <sub>2</sub> O <sub>6</sub> SrU, Ba <sub>2</sub> O <sub>6</sub> SrW, Ba <sub>2</sub> O <sub>6</sub> TiZr, Ba <sub>9</sub> O <sub>24</sub> Sc <sub>2</sub> Si <sub>6</sub> , BeF <sub>4</sub> Li <sub>2</sub> , BiCsF <sub>6</sub> , BiF <sub>6</sub> Li, BiF <sub>6</sub> Na, BiF <sub>6</sub> Rb, BiI <sub>3</sub> , BiNaO <sub>3</sub> , Bi <sub>2</sub> Si <sub>2</sub> Te <sub>6</sub> , Br <sub>14</sub> Re <sub>6</sub> Te <sub>14</sub> , BrCsF <sub>6</sub> , Br <sub>3</sub> Pt, Br <sub>6</sub> W, CCs <sub>2</sub> I <sub>18</sub> Zr <sub>7</sub> , Cl <sub>12</sub> Zr <sub>6</sub> , C <sub>2</sub> MgNa <sub>2</sub> O <sub>6</sub> , CaF <sub>6</sub> Pd, CaF <sub>6</sub> Pt, CaF <sub>6</sub> Si, CaF <sub>6</sub> Sn, CaO <sub>3</sub> Sn, Ca <sub>2</sub> Hf <sub>7</sub> O <sub>16</sub> , Ca <sub>3</sub> O <sub>6</sub> U, CdF <sub>6</sub> Pd, CdF <sub>6</sub> Pt, CdF <sub>6</sub> Sn, CdF <sub>6</sub> Ti, CdGeO <sub>3</sub> , CdO <sub>3</sub> S, CdO <sub>3</sub> Sn, CdO <sub>3</sub> Ti, Cd <sub>2</sub> P <sub>2</sub> Se <sub>6</sub> , Cl <sub>12</sub> NSC <sub>7</sub> , Cl <sub>18</sub> Cs <sub>2</sub> Nb <sub>6</sub> Pb, Cl <sub>18</sub> Cs <sub>2</sub> PbTa <sub>6</sub> , Cl <sub>18</sub> K <sub>2</sub> Nb <sub>6</sub> Sn, Cl <sub>2</sub> Pd, Cl <sub>3</sub> Pt, Cl <sub>3</sub> Sc, Cl <sub>6</sub> W, Cl <sub>8</sub> O <sub>12</sub> Si <sub>8</sub> , CsF <sub>6</sub> Nb, CsF <sub>6</sub> Sb, CsO <sub>8</sub> Te <sub>3</sub> Y, Cs <sub>2</sub> I <sub>6</sub> O <sub>18</sub> Zr, Cs <sub>8</sub> OTl <sub>8</sub> , FKO <sub>6</sub> Te <sub>3</sub> , F <sub>31</sub> Rb <sub>7</sub> Th <sub>6</sub> , F <sub>3</sub> N <sub>3</sub> S <sub>3</sub> , F <sub>6</sub> LiNb, F <sub>6</sub> LiSb, F <sub>6</sub> LiTa, F <sub>6</sub> MgPb, F <sub>6</sub> PbZn, F <sub>6</sub> PdZn, F <sub>6</sub> PtZn, F <sub>6</sub> RbSb, F <sub>6</sub> SnZn, Ge, GeMgO <sub>3</sub> , GeO <sub>3</sub> Pb, GeO <sub>3</sub> Zn, GeO <sub>4</sub> Zn <sub>2</sub> , Ge <sub>2</sub> In <sub>2</sub> Te <sub>6</sub> , HfTe <sub>4</sub> Tl <sub>4</sub> , I <sub>3</sub> InO <sub>9</sub> , I <sub>3</sub> O <sub>9</sub> Sc, I <sub>3</sub> O <sub>9</sub> Tl, I <sub>3</sub> Sb, I <sub>3</sub> Y, I <sub>6</sub> K <sub>2</sub> O <sub>18</sub> Zr, I <sub>6</sub> O <sub>18</sub> Rb <sub>2</sub> Zr, In <sub>6</sub> O <sub>12</sub> Te, In <sub>6</sub> O <sub>12</sub> W, La <sub>4</sub> O <sub>12</sub> Ti <sub>3</sub> , La <sub>6</sub> O <sub>12</sub> U, Li <sub>16</sub> N <sub>8</sub> Nb <sub>2</sub> O, Li <sub>16</sub> N <sub>8</sub> OTa <sub>2</sub> , LiNbO <sub>3</sub> , LiS <sub>2</sub> Sb, Li <sub>2</sub> O <sub>4</sub> Se, Li <sub>2</sub> O <sub>4</sub> W, Li <sub>6</sub> O <sub>6</sub> Te, Li <sub>6</sub> O <sub>6</sub> U, Li <sub>8</sub> O <sub>6</sub> Pb, Li <sub>8</sub> O <sub>6</sub> Pt, Li <sub>8</sub> O <sub>6</sub> Sn, Lu <sub>6</sub> O <sub>12</sub> U, MgO <sub>13</sub> Te <sub>6</sub> , MgO <sub>3</sub> Ti, Mg <sub>2</sub> P <sub>2</sub> Se <sub>6</sub> , Mg <sub>3</sub> O <sub>6</sub> Te, Mo <sub>18</sub> S <sub>22</sub> Tl <sub>4</sub> , Mo <sub>3</sub> S <sub>4</sub> , Mo <sub>3</sub> Se <sub>4</sub> , Mo <sub>6</sub> S <sub>8</sub> ,

Part 17 of all the predicted materials with band crossings from **Cases 1 or 2:**

148	<chem>NaNbO3</chem> , <chem>NaO3Sb</chem> , <chem>Na8O18Si7</chem> , <chem>Nb6O12Ti2</chem> , <chem>O12TeTl6</chem> , <chem>O12TeY6</chem> , <chem>O12UY6</chem> , <chem>O12WY6</chem> , <chem>O2Si</chem> , <chem>O3SbTl</chem> , <chem>O3SiZn</chem> , <chem>O3SnZn</chem> , <chem>O3TiZn</chem> , <chem>O4SiZn2</chem> , <chem>O6TeTl6</chem> , <chem>O9Te4</chem> , <chem>P2S6Sn2</chem> , <chem>S</chem> , <chem>S6</chem> , <chem>Se6</chem> , <chem>Si</chem> ,
149	<chem>As2CaO6</chem> , <chem>GeI6Rb</chem> , <chem>GeO6SrTe</chem> , <chem>OTi3</chem> , <chem>O6PbSb2</chem> ,
150	<chem>AlCaF6Na</chem> , <chem>AlF3</chem> , <chem>AlF6LiMg</chem> , <chem>As2Cl9Cs3</chem> , <chem>As2O14Pb3TeZn3</chem> , <chem>B2Ga2K2O7</chem> , <chem>BaGe4O9</chem> , <chem>Ba3Ga2Ge4O14</chem> , <chem>Ba3Ga3NbO14Si2</chem> , <chem>Bi2Cl9Cs3</chem> , <chem>Ca3Ga3O14Si2Ta</chem> , <chem>Cl9Cs3Sb2</chem> , <chem>Cs2O3Te</chem> , <chem>F6GeLi2</chem> , <chem>F6GeNa2</chem> , <chem>F6K2U</chem> , <chem>F6Li2Si</chem> , <chem>F6Na2Pt</chem> , <chem>F6Na2Th</chem> , <chem>F6Na2U</chem> , <chem>Ga2Ge4O14Pb3</chem> , <chem>Ga3NbO14Si2Sr3</chem> , <chem>Ga3O14Si2Sr3Ta</chem> , <chem>Ga5La3O14Sn</chem> , <chem>Ge4O9Pb</chem> , <chem>Ge4O9Sr</chem> , <chem>In2O6Te</chem> , <chem>K2O6S2</chem> , <chem>La2O3</chem> , <chem>O6Rb2S2</chem> , <chem>O6Sc2Te</chem> , <chem>O6TeTl2</chem> ,
151	<chem>Cl3Ti</chem> , <chem>Li5O6Re</chem> ,
152	<chem>AgPb4Pd6</chem> , <chem>AlAsO4</chem> , <chem>AsBO4</chem> , <chem>AsGaO4</chem> , <chem>BF4Li</chem> , <chem>BO5PSr</chem> , <chem>B2O3</chem> , <chem>B7Cs3Li4O14</chem> , <chem>BaO2Zn</chem> , <chem>BeF2</chem> , <chem>CdTe</chem> , <chem>GeO2</chem> , <chem>HgO</chem> , <chem>HgS</chem> , <chem>HgTe</chem> , <chem>Hg3O6S</chem> , <chem>K2P2Se6</chem> , <chem>Li2O4SiSr</chem> , <chem>O2Si</chem> , <chem>O2Ti</chem> , <chem>P2Rb2Se6</chem> , <chem>Se</chem> , <chem>TeZn</chem> ,
154	<chem>AlO4P</chem> , <chem>HgO</chem> , <chem>HgO2Sr</chem> , <chem>HgS</chem> , <chem>O23S5Te4</chem> , <chem>S</chem> , <chem>Te</chem> ,
155	<chem>AlF3</chem> , <chem>Al2B2BaO7</chem> , <chem>Al2BaO7Sb2</chem> , <chem>Al7Te10</chem> , <chem>AsF7Sn</chem> , <chem>BBe2CsF2O3</chem> , <chem>BBe2F2KO3</chem> , <chem>C4CaMg3O12</chem> , <chem>Ca3Na2O9Ta2</chem> , <chem>F3Sc</chem> , <chem>Ga3InTe5</chem> , <chem>Ga3NaTe5</chem> , <chem>Ga7Te10</chem> , <chem>In7Te10</chem> , <chem>O2Si</chem> , <chem>O8RbS2Tl</chem> ,
156	<chem>AgAlS2</chem> , <chem>Ag6ClF3Mo2O7</chem> , <chem>AlF6K2Li</chem> , <chem>BBeLi</chem> , <chem>BiTe</chem> , <chem>Br7Nb3S</chem> , <chem>CSi</chem> , <chem>CdGaInS4</chem> , <chem>CdI2</chem> , <chem>I2Pb</chem> , <chem>I7Nb3Te</chem> , <chem>InLiMo3O8</chem> , <chem>In2S6Zn3</chem> , <chem>LiMo3O8Sc</chem> , <chem>LiMo3O8Y</chem> , <chem>SZn</chem> , <chem>Sb2Te3</chem> ,
157	<chem>As5Cs3O9</chem> , <chem>Au6Cs4S5</chem> , <chem>Bi2Pt</chem> ,
158	<chem>F6O4P4</chem> ,
159	<chem>AgBa7Ga5Se15</chem> , <chem>AIKO4Si</chem> , <chem>Ba3MoN4</chem> , <chem>Bi2O3</chem> , <chem>Br6Cl8Cs2Mo6</chem> , <chem>Br6Cl8Cs2W6</chem> , <chem>C3N4</chem> , <chem>Ge3N4</chem> , <chem>K5NaSe27Ti6</chem> , <chem>Mo3O12SeTl2</chem> , <chem>N4Si3</chem> , <chem>O12Rb2TeW3</chem> , <chem>OTi6</chem> ,
160	<chem>AgNO3</chem> , <chem>Al2MgS4</chem> , <chem>Al2MgSe4</chem> , <chem>Al2S4Zn</chem> , <chem>AsS3Tl3</chem> , <chem>AsSe3Tl3</chem> , <chem>As2Sn2Sr</chem> , <chem>As2Te3</chem> , <chem>As4Pb9S15</chem> , <chem>BN</chem> , <chem>B3Be3F4NaO9Sr3</chem> , <chem>BaO3Ti</chem> , <chem>Be3N2</chem> , <chem>Bi2Ge3Te6</chem> , <chem>Bi2O3</chem> , <chem>Bi2Te3</chem> , <chem>BrCsO3</chem> , <chem>BrKO3</chem> , <chem>BrO3Rb</chem> , <chem>BrO3Tl</chem> , <chem>Br3CsGe</chem> , <chem>CAgN</chem> , <chem>CCs4O4</chem> , <chem>CIN</chem> , <chem>CLi4O4</chem> , <chem>CNa4O4</chem> , <chem>COS</chem> , <chem>CO4Rb4</chem> , <chem>C3Al4</chem> , <chem>C3Al6N2</chem> , <chem>C3N4</chem> , <chem>C5Al4Zr2</chem> , <chem>C6Al4Zr3</chem> , <chem>Ca3O5Si</chem> , <chem>Cd4K6Se13Sn3</chem> , <chem>CIKO3</chem> , <chem>ClO3Rb</chem> , <chem>ClO3Tl</chem> , <chem>Cl2Zr</chem> , <chem>Cl3CsGe</chem> , <chem>Cl8Na2Ti3</chem> , <chem>CsGeI3</chem> , <chem>F4OU</chem> , <chem>GaSe</chem> , <chem>GeTe</chem> , <chem>IKO3</chem> , <chem>IO3Rb</chem> , <chem>I3S24Sb</chem> , <chem>InSe</chem> , <chem>In2S5Zn2</chem> , <chem>In2Se3</chem> , <chem>In3O12Sb5</chem> , <chem>KNbO3</chem> , <chem>Li5NaSn4</chem> , <chem>MoS2</chem> , <chem>MoSe2</chem> , <chem>N3Na</chem> , <chem>Nb2O6Pb</chem> , <chem>PbS</chem> , <chem>SZn</chem> , <chem>S2Ta</chem> , <chem>S2W</chem> , <chem>S3SbTl3</chem> , <chem>S3Ti</chem> , <chem>Sb2Se2Te</chem> , <chem>Se2Ta</chem> ,
161	<chem>AgNO3</chem> , <chem>AgO3Ta</chem> , <chem>Ag2Nb4O11</chem> , <chem>Ag3AsS3</chem> , <chem>Ag3AsSe3</chem> , <chem>Ag3NO3Se</chem> , <chem>Ag3S3Sb</chem> , <chem>AlBiO3</chem> , <chem>B2BaO6Zr</chem> , <chem>B7ClO13Zn3</chem> , <chem>B9BaNaO15</chem> , <chem>B9LiO15Sr</chem> , <chem>BiCs2Mo3NaO12</chem> , <chem>Br4Ga2</chem> , <chem>CdCl6KRb3</chem> , <chem>CdF3Na</chem> , <chem>Cl3LuO12</chem> , <chem>CsF3Pb</chem> , <chem>GaLaO3</chem> , <chem>Ga2I4</chem> , <chem>GeO3Zn</chem> , <chem>Ge3La4S12</chem> , <chem>I4InRb</chem> , <chem>K3SbSe4</chem> , <chem>LiO3Ta</chem> , <chem>NaNbO3</chem> , <chem>O10P4</chem> , <chem>O3PbZn</chem> , <chem>O3SnZn</chem> , <chem>O3TiZn</chem> , <chem>O5P2</chem> , <chem>Pd8Sb3</chem> , <chem>Si38Te16</chem> ,
162	<chem>As2CdO6</chem> , <chem>As2HgO6</chem> , <chem>As2Hg2O6</chem> , <chem>As2O6Sr</chem> , <chem>Au7IP10</chem> , <chem>BaO6Sb2</chem> , <chem>BiI3</chem> , <chem>CdO6Sb2</chem> , <chem>Cl3Ti</chem> , <chem>Cl4Mo</chem> , <chem>F6HfLi2</chem> ,

Part 18 of all the predicted materials with band crossings from **Cases 1 or 2:**

162	<chem>F6Li2Zr</chem> , <chem>In4O7Rb2</chem> , <chem>K2Mg2O7Si2</chem> , <chem>O6PbSb2</chem> , <chem>O6Sb2Sr</chem> , <chem>O8Ta2U</chem> ,
163	<chem>AgGaP2Se6</chem> , <chem>AgInP2Se6</chem> , <chem>AgP2S6Sc</chem> , <chem>AgP2ScSe6</chem> , <chem>Ag5HgO6Sb</chem> , <chem>AlCaF6Li</chem> , <chem>AlF6LiSr</chem> , <chem>Al2B2Na2O7</chem> , <chem>Br6Na3Sc</chem> , <chem>CaF6GaLi</chem> , <chem>Cl18CsLuNb6</chem> , <chem>Cl6InNa3</chem> , <chem>Cs2I14Mo6</chem> , <chem>GeNa2O6Te</chem> , <chem>I6Li2U</chem> , <chem>I6PbTh</chem> , <chem>I6SnTh</chem> , <chem>O2Si</chem> , <chem>O3SbTl</chem> , <chem>Pt3Tl2</chem> ,
164	<chem>Ac2O3</chem> , <chem>AgBiS2</chem> , <chem>AgBiSe2</chem> , <chem>AgScSe2</chem> , <chem>Ag2BaS2</chem> , <chem>AlCsMo2O8</chem> , <chem>AllaSi2</chem> , <chem>AlMo2O8Tl</chem> , <chem>Al2CaGe2</chem> , <chem>Al2CaSi2</chem> , <chem>Al2Cs2O7Sb2</chem> , <chem>Al2Ge2Sr</chem> , <chem>Al2K2O7Sb2</chem> , <chem>Al2MgSi2</chem> , <chem>Al2Mg2Se5</chem> , <chem>Al2O7Rb2Sb2</chem> , <chem>Al2Si2Sr</chem> , <chem>As2BaCd2</chem> , <chem>As2BaMg2</chem> , <chem>As2Be2Ca</chem> , <chem>As2Be2Mg</chem> , <chem>As2CaCd2</chem> , <chem>As2CaMg2</chem> , <chem>As2CaZn2</chem> , <chem>As2Cd2Sr</chem> , <chem>As2Ge2Te5</chem> , <chem>As2LaLi3</chem> , <chem>As2Mg2Sr</chem> , <chem>As2Mg2Zn</chem> , <chem>As2Mg3</chem> , <chem>As2SrZn2</chem> , <chem>Au3Cs2</chem> , <chem>Au3CsSe2</chem> , <chem>Au3RbSe2</chem> , <chem>BN</chem> , <chem>BaBi2Mg2</chem> , <chem>BaCd2P2</chem> , <chem>BaCd2Sb2</chem> , <chem>BaMgO8Si2Sr2</chem> , <chem>BaMg2P2</chem> , <chem>BaMg2Sb2</chem> , <chem>BaSn2</chem> , <chem>Ba3MgO9Ta2</chem> , <chem>Ba3Nb2O9Zn</chem> , <chem>Ba3O9SrTa2</chem> , <chem>Ba5Nb4O15</chem> , <chem>Be</chem> , <chem>Be2CaP2</chem> , <chem>Be2MgN2</chem> , <chem>Be2MgP2</chem> , <chem>Be3N2</chem> , <chem>Bi2Br9Cs3</chem> , <chem>Bi2CaMg2</chem> , <chem>Bi2LaLi3</chem> , <chem>Bi2Li3Y</chem> , <chem>Bi2Mg2Sr</chem> , <chem>Bi2Pb2Se5</chem> , <chem>BrNZr</chem> , <chem>Br2Ti</chem> , <chem>Br6Na2U</chem> , <chem>Br9Cs3Sb2</chem> , <chem>CN2O2Y2</chem> , <chem>CNb2S2</chem> , <chem>CS2Ta2</chem> , <chem>C2Al2Mg</chem> , <chem>C2Na2Pd</chem> , <chem>C2Na2Pt</chem> , <chem>C8B2N8Zn</chem> , <chem>CaCd2P2</chem> , <chem>CaCd2Sb2</chem> , <chem>CaGe2</chem> , <chem>CaI2</chem> , <chem>CaMg2N2</chem> , <chem>CaMg2Sb2</chem> , <chem>CaP2Zn2</chem> , <chem>CaSi2</chem> , <chem>Ca2GeO4</chem> , <chem>Ca2O4Si</chem> , <chem>Ca3N2</chem> , <chem>CdI2</chem> , <chem>CdO4S</chem> , <chem>Cd2P2Sr</chem> , <chem>Cd2Sb2Sr</chem> , <chem>CINZr</chem> , <chem>Cl2Mg</chem> , <chem>Cl6Cs2Th</chem> , <chem>Cl6Cs2U</chem> , <chem>Cl6Na2U</chem> , <chem>Cl6U</chem> , <chem>Cl9Cs3Sb2</chem> , <chem>Cs2F6Hf</chem> , <chem>Cs2F6Pt</chem> , <chem>Cs2F6Sn</chem> , <chem>Cs2F6Zr</chem> , <chem>Cs3I9Sb2</chem> , <chem>F3OP</chem> , <chem>F6GeNa2</chem> , <chem>F6Hg3S2Si</chem> , <chem>F6K2Pt</chem> , <chem>F6K2Ti</chem> , <chem>F6Na2Si</chem> , <chem>F6Na2Ti</chem> , <chem>F6PtRb2</chem> , <chem>F6Rb2Zr</chem> , <chem>F6S</chem> , <chem>F6SnTl2</chem> , <chem>F6TiTl2</chem> , <chem>Ga2I2Y2</chem> , <chem>GeI2</chem> , <chem>GeI2La2</chem> , <chem>GeSb4Te7</chem> , <chem>Ge2Sr</chem> , <chem>HfS2</chem> , <chem>HfSe2</chem> , <chem>Hf2N2S</chem> , <chem>HgPt2Se3</chem> , <chem>I2Mg</chem> , <chem>I2Zn</chem> , <chem>In2Se3</chem> , <chem>KMo2O8Sc</chem> , <chem>K2Li4O6U</chem> , <chem>K3NaO8Se2</chem> , <chem>K4O12Zr5</chem> , <chem>LaLi3P2</chem> , <chem>LaLi3Sb2</chem> , <chem>La2O2Se</chem> , <chem>La2O3</chem> , <chem>Li2N2Zr</chem> , <chem>Li2SiZn</chem> , <chem>Lu2O2S</chem> , <chem>Lu2O3</chem> , <chem>Mg2N2Sr</chem> , <chem>Mg2Sb2Sr</chem> , <chem>Mg3Sb2</chem> , <chem>MoO4Tl2</chem> , <chem>Mo2O8ScTl</chem> , <chem>N2SZr2</chem> , <chem>N2SeTh2</chem> , <chem>NaO6S2Tl3</chem> , <chem>NaO8Rb3W2</chem> , <chem>O2Pt</chem> , <chem>O2SY2</chem> , <chem>O3Sc2</chem> , <chem>O3U</chem> , <chem>O3Y2</chem> , <chem>P2SrZn2</chem> , <chem>PdTe2</chem> , <chem>Pd4Se6Tl2</chem> , <chem>PtSe2</chem> , <chem>PtTe2</chem> , <chem>Pt3U</chem> , <chem>Pt4S6Tl2</chem> , <chem>Pt4Se6Tl2</chem> , <chem>Pt4Te6Tl2</chem> , <chem>S2Sn</chem> , <chem>S2Ti</chem> , <chem>S2Zr</chem> , <chem>Sb2Te</chem> , <chem>Se2Sn</chem> , <chem>Se2Zr</chem> , <chem>Te2Ti</chem> , <chem>Te6Zr5</chem> ,
165	<chem>Al2O8Si2Sr</chem> , <chem>Ba3Bi2O9Te</chem> , <chem>F18InSb3</chem> , <chem>F3La</chem> , <chem>F3Y</chem> , <chem>F6Li3Sc</chem> , <chem>Ge3O9Rb2Ti</chem> , <chem>InKO8W2</chem> , <chem>InLi3O3</chem> , <chem>LiTe3</chem> , <chem>Mg4Nb2O9</chem> , <chem>Mg4O9Ta2</chem> , <chem>NaTe3</chem> , <chem>Nb2O9Zn4</chem> ,
166	<chem>AgAsSe2</chem> , <chem>AgBiSe2</chem> , <chem>AgBiTe2</chem> , <chem>AgGeLi2</chem> , <chem>AgInO2</chem> , <chem>AgInS2</chem> , <chem>AgLuO2</chem> , <chem>AgO2Sc</chem> , <chem>AgSbTe2</chem> , <chem>Ag3As2K3</chem> , <chem>AlCaF14Mg3Na3</chem> , <chem>AlCs2F6Na</chem> , <chem>AlF6K2Li</chem> , <chem>AllaO3</chem> , <chem>AlliO2</chem> , <chem>AlNaO2</chem> , <chem>AlO2Tl</chem> , <chem>Al2MgS4</chem> , <chem>Al3Cs2F12Na</chem> , <chem>As</chem> , <chem>AsB6</chem> , <chem>AsCa2I</chem> , <chem>AsF6K</chem> , <chem>AsNaTe2Zr2</chem> , <chem>As2B12</chem> , <chem>As2Ba3O8</chem> , <chem>As2BeK4</chem> , <chem>As2CaGa2</chem> , <chem>As2CdK4</chem> , <chem>As2GeTe4</chem> , <chem>As2HgK4</chem> , <chem>As2K4Zn</chem> , <chem>As2Te3</chem> , <chem>As3Cd4K</chem> , <chem>AuF6K</chem> , <chem>Au3K3Sb2</chem> , <chem>Au3Rb3Sb2</chem> , <chem>B</chem> , <chem>B12</chem> , <chem>B12P2</chem> , <chem>B12S</chem> , <chem>B12Si3</chem> , <chem>BS2Tl</chem> , <chem>B2Ba2MgO6</chem> , <chem>B2Mo</chem> , <chem>B4Mo2</chem> , <chem>B6O</chem> , <chem>B6P</chem> , <chem>B9MgN</chem> , <chem>BaF6Ge</chem> , <chem>BaF6Pb</chem> , <chem>BaF6Ti</chem> , <chem>BaGe2Li2Mg2</chem> , <chem>BaHgO2</chem> , <chem>BaLi2Mg2Si2</chem> , <chem>BaO3Si</chem> , <chem>Ba2BrN</chem> , <chem>Ba2CIN</chem> , <chem>Ba2CIP</chem> , <chem>Ba2FN</chem> , <chem>Ba2Mg17</chem> , <chem>Ba3Nb2O8</chem> , <chem>Ba3O9Sc4</chem> , <chem>Ba8O24Re2W3</chem> , <chem>BeK4P2</chem> , <chem>Be2F8K2Pb</chem> , <chem>Be2F8K2Sr</chem> , <chem>Bi</chem> , <chem>BiKLi6O6</chem> , <chem>BiRbS2</chem> , <chem>BiS2Tl</chem> , <chem>BiSe2Tl</chem> , <chem>BiTe2Tl</chem> , <chem>Bi2Se2Te</chem> , <chem>BrCa2N</chem> , <chem>BrHfN</chem> , <chem>BrLa</chem> , <chem>BrNSr2</chem> , <chem>BrNZr</chem> , <chem>Br2Ca3Si</chem> , <chem>Br2Cd</chem> , <chem>Br2Zn</chem> , <chem>Br7In4</chem> , <chem>C</chem> , <chem>CAIOSc</chem> , <chem>CB4</chem> , <chem>CCl2Lu2</chem> , <chem>CMgN2</chem> , <chem>CS14</chem> , <chem>CS2Ta2</chem> , <chem>CY2</chem> , <chem>C2Ca</chem> , <chem>C2CaK2O6</chem> , <chem>C2K2MgO6</chem> , <chem>C3Al4</chem> , <chem>C3B12</chem> , <chem>C5Tis</chem> , <chem>C6Al4Hf3</chem> , <chem>CaF6Ti</chem> , <chem>CaGe2</chem> , <chem>CaHgO2</chem> , <chem>CaO4U</chem> , <chem>CaSi2</chem> , <chem>Ca2CIN</chem> , <chem>Ca2F4</chem> , <chem>Ca2IP</chem> , <chem>Ca2O8Pt3</chem> , <chem>CdCl2</chem> , <chem>CdNa4P2</chem> , <chem>CdO4U</chem> , <chem>ClHFN</chem> , <chem>ClLa</chem> , <chem>ClLi4N</chem> , <chem>ClMg2N</chem> , <chem>CINSr2</chem> , <chem>CINZr</chem> , <chem>ClOY</chem> , <chem>ClSc</chem> , <chem>ClY</chem> , <chem>Cl2CsI</chem> , <chem>Cl2CsKO8</chem> ,

Part 19 of all the predicted materials with band crossings from **Cases 1 or 2:**

166	<chem>Cl2Li5N</chem> , <chem>Cl2Mg</chem> , <chem>Cl2Pt</chem> , <chem>Cl3Re</chem> , <chem>Cl8Na2Ti3</chem> , <chem>Cl9Re3</chem> , <chem>CsLaS2</chem> , <chem>CsLuS2</chem> , <chem>Cs2F6GaN</chem> , <chem>Cs2F6NaTi</chem> , <chem>Cs2O</chem> , <chem>Cs2O12Te4</chem> , <chem>Cs2Pt4Se6</chem> , <chem>Cs4F12Ga2KLi</chem> , <chem>FLaO</chem> , <chem>FLuS</chem> , <chem>FNTh</chem> , <chem>FOY</chem> , <chem>F2O2U</chem> , <chem>F6GaLiRb2</chem> , <chem>F6PbPt</chem> , <chem>F6SbTl</chem> , <chem>Ga</chem> , <chem>GaGeTe</chem> , <chem>GaLiO2</chem> , <chem>GaO2Tl</chem> , <chem>GaP</chem> , <chem>GaS</chem> , <chem>GeI2La2</chem> , <chem>GeI2Y2</chem> , <chem>HfIN</chem> , <chem>HfN2Sr</chem> , <chem>Hg</chem> , <chem>HgK4P2</chem> , <chem>HgNa4P2</chem> , <chem>HgO2Sr</chem> , <chem>INSr2</chem> , <chem>INZr</chem> , <chem>I2La2Te</chem> , <chem>I2Zn</chem> , <chem>I8Nb3</chem> , <chem>InKO2</chem> , <chem>InK5Pb8</chem> , <chem>InLiSe2</chem> , <chem>InMg3</chem> , <chem>InNaS2</chem> , <chem>InNaSe2</chem> , <chem>InP3</chem> , <chem>InS2Tl</chem> , <chem>In2Te3</chem> , <chem>KLaO2</chem> , <chem>KLaS2</chem> , <chem>KLaTe2</chem> , <chem>KLi6O6Ta</chem> , <chem>KLuS2</chem> , <chem>KO2Sc</chem> , <chem>KO2Tl</chem> , <chem>KO2Y</chem> , <chem>KO3Pd2</chem> , <chem>KS2Y</chem> , <chem>KTe2Y</chem> , <chem>K2O3Sn2</chem> , <chem>K2O8PbS2</chem> , <chem>K2Pt4S6</chem> , <chem>K2Pt4Se6</chem> , <chem>K4P2Zn</chem> , <chem>LaNaSe2</chem> , <chem>LaO12Sb5</chem> , <chem>LaO2Rb</chem> , <chem>LaRbS2</chem> , <chem>LaRbSe2</chem> , <chem>LiS2Sc</chem> , <chem>LiS2Y</chem> , <chem>LiSe2Y</chem> , <chem>Li2O</chem> , <chem>Li4Mo3O8</chem> , <chem>Li4P2Sr</chem> , <chem>Li6O6U</chem> , <chem>Li8Pb3</chem> , <chem>LuNaS2</chem> , <chem>LuO2Rb</chem> , <chem>LuRbS2</chem> , <chem>LuRbSe2</chem> , <chem>LuS2Tl</chem> , <chem>LuSe2Tl</chem> , <chem>LuTe2Tl</chem> , <chem>MgN2Si</chem> , <chem>MgO</chem> , <chem>N2NaNb</chem> , <chem>N2NaTa</chem> , <chem>N2SrZr</chem> , <chem>N2W</chem> , <chem>N3Na</chem> , <chem>N4Th3</chem> , <chem>NaO2Sc</chem> , <chem>NaO2Tl</chem> , <chem>NaS2Sc</chem> , <chem>NaS2Y</chem> , <chem>NaSe2Y</chem> , <chem>Nb6Zn7</chem> , <chem>OPYZn</chem> , <chem>OTl2</chem> , <chem>O2</chem> , <chem>O2RbSc</chem> , <chem>O2RbTl</chem> , <chem>O2RbY</chem> , <chem>O3Rb2Sn2</chem> , <chem>O4SrU</chem> , <chem>P</chem> , <chem>Pd3S2Tl2</chem> , <chem>Pt2Te3</chem> , <chem>Pt3Te4</chem> , <chem>Pt4Rb2Se6</chem> , <chem>RbS2Y</chem> , <chem>STi</chem> , <chem>S2TIY</chem> , <chem>Sb</chem> , <chem>ScTe2Tl</chem> , <chem>SeTi</chem> , <chem>Se2TIY</chem> , <chem>Ta6Zn7</chem> , <chem>TeZr3</chem> , <chem>Te2TIY</chem> ,
167	<chem>AgHg3O6Sb</chem> , <chem>AgO3Ta</chem> , <chem>Ag2Nb4O11</chem> , <chem>Ag2O11Ta4</chem> , <chem>Ag5IO6</chem> , <chem>AlBO3</chem> , <chem>AlF3</chem> , <chem>Al2B2CaO7</chem> , <chem>Al2O3</chem> , <chem>Al3As5Ba3</chem> , <chem>Al3Ba3P5</chem> , <chem>Al3Bi5Br12</chem> , <chem>Al3Bi5Cl12</chem> , <chem>Al6Ge5</chem> , <chem>As3CsO12Zr2</chem> , <chem>As3KO12Zr2</chem> , <chem>As3LiO12Zr2</chem> , <chem>As3NaO12Ti2</chem> , <chem>As3NaO12Zr2</chem> , <chem>AuK3Se2</chem> , <chem>AuNa3S2</chem> , <chem>Au3F12La</chem> , <chem>BBe2F2KO3</chem> , <chem>BGaO3</chem> , <chem>BInO3</chem> , <chem>BNaO2</chem> , <chem>BO3Sc</chem> , <chem>B2Ca3O6</chem> , <chem>B2Hg3O6</chem> , <chem>B3K3O6</chem> , <chem>B3K3S6</chem> , <chem>B3Na3O6</chem> , <chem>B3Na3S6</chem> , <chem>B3Rb3S6</chem> , <chem>Ba2Re6S11</chem> , <chem>Ba3BeCl18Zr6</chem> , <chem>Ba3BiNaO6</chem> , <chem>Ba3Ga3P5</chem> , <chem>Ba3NaNbO6</chem> , <chem>Ba3NaO6Sb</chem> , <chem>Ba3NaO6Ta</chem> , <chem>Ba3O9W2</chem> , <chem>Ba4O6Pt</chem> , <chem>Ba6O18W4</chem> , <chem>BiNaO6Sr3</chem> , <chem>Bi5Cl12Ga3</chem> , <chem>Br4ORb6</chem> , <chem>Br6CdRb4</chem> , <chem>Br6Cs4Pb</chem> , <chem>Br6PbRb4</chem> , <chem>Br9Cs3Y2</chem> , <chem>CCdO3</chem> , <chem>CMgO3</chem> , <chem>CO2</chem> , <chem>CO3Zn</chem> , <chem>C4K2N4Zn</chem> , <chem>Ca14Si19</chem> , <chem>Ca3N2</chem> , <chem>Ca4O6Pd</chem> , <chem>Ca4O6Pt</chem> , <chem>CdCl6K4</chem> , <chem>CdCl6Rb4</chem> , <chem>CdO6PtSr3</chem> , <chem>Cd2Mo15Se19</chem> , <chem>ClCs8Ga11</chem> , <chem>Cl4Cs6O</chem> , <chem>Cl4ORb6</chem> , <chem>Cl6Cs4Pb</chem> , <chem>Cl9Cs3In2</chem> , <chem>Cl9Cs3Lu2</chem> , <chem>Cl9Cs3Sc2</chem> , <chem>Cl9Cs3Tl2</chem> , <chem>Cl9Cs3Y2</chem> , <chem>Cl9In5</chem> , <chem>CsN3O11U</chem> , <chem>F3Ga</chem> , <chem>F3In</chem> , <chem>F3Sc</chem> , <chem>GaLaO3</chem> , <chem>Ga2O3</chem> , <chem>Ge3Hf2Na4O12</chem> , <chem>HeO2Si</chem> , <chem>In2O3</chem> , <chem>In2S3</chem> , <chem>K2O11Ta4</chem> , <chem>LiNO3</chem> , <chem>LiNbO3</chem> , <chem>LiNbO6Sr3</chem> , <chem>LiO6SbSr3</chem> , <chem>LiO6Sr3Ta</chem> , <chem>Lu2S3</chem> , <chem>MgO6PtSr3</chem> , <chem>Mo15Se19</chem> , <chem>Mo15Se19Tl2</chem> , <chem>NNaO3</chem> , <chem>N2</chem> , <chem>NaNbO6Sr3</chem> , <chem>NaO6SbSr3</chem> , <chem>NaO6Sr3Ta</chem> , <chem>Na2Nb4O11</chem> , <chem>Na2O11Ta4</chem> , <chem>Na4O12Si3Sn2</chem> , <chem>Na4O12Si3Zr2</chem> , <chem>O2Si</chem> , <chem>O3Te</chem> , <chem>O6PdSr4</chem> , <chem>O6PtSr3Zn</chem> , <chem>O6PtSr4</chem> , <chem>Pd8Sb3</chem> , <chem>Re6S11Sr2</chem> ,
169	<chem>AlInS3</chem> , <chem>AlInSe3</chem> , <chem>AlNaO4Si</chem> , <chem>Al2S3</chem> , <chem>GaInS3</chem> , <chem>GaInSe3</chem> , <chem>In2Se3</chem> ,
170	<chem>In2Se3</chem> ,
173	<chem>AgLa3Se7Si</chem> , <chem>AgLa3Se7Sn</chem> , <chem>AlCdLa3S7</chem> , <chem>AlGeKO4</chem> , <chem>All3O9</chem> , <chem>Alla3MgS7</chem> , <chem>Alla3S7Zn</chem> , <chem>AlNaO4Si</chem> , <chem>Al2BaO4</chem> , <chem>Al2CaO4</chem> , <chem>Al2O4Sr</chem> , <chem>AsNaO4Zn</chem> , <chem>AsO4Tl3</chem> , <chem>As3ClO9Pb5</chem> , <chem>B2Bi2O7Sr</chem> , <chem>Ba4ClGe3NaS10</chem> , <chem>BeLa3S7Sc</chem> , <chem>Br3KTi</chem> , <chem>Cl14Sn2W3</chem> , <chem>Cs2I4O11</chem> , <chem>Cs2Mo3O12Se</chem> , <chem>Cs2Mo3O12Te</chem> , <chem>Cs2O12SeW3</chem> , <chem>F10NaSb3</chem> , <chem>GaI3O9</chem> , <chem>GaNaO4Si</chem> , <chem>I3InO9</chem> , <chem>I3P</chem> , <chem>KLiMoO4</chem> , <chem>LaO3Tl</chem> , <chem>N4P2Sr</chem> , <chem>N4Si3</chem> , <chem>NaS7SiY3</chem> ,
174	<chem>Ag5RbS3</chem> , <chem>BCdLiO3</chem> , <chem>Ba7Cl2F12</chem> , <chem>Br2F12Pb7</chem> , <chem>C12N16</chem> , <chem>CLiNaO3</chem> , <chem>C6N8</chem> , <chem>Cl2F12Pb7</chem> , <chem>GaSe</chem> , <chem>Ga9O2S13Tl3</chem> , <chem>K2O9Si3Zr</chem> , <chem>Li2O2</chem> ,

Part 20 of all the predicted materials with band crossings from **Cases 1 or 2:**

	AcBr <sub>3</sub> , AcCl <sub>3</sub> , Al <sub>6</sub> B <sub>5</sub> F <sub>3</sub> O <sub>15</sub> , As <sub>3</sub> Ca <sub>2</sub> ClO <sub>12</sub> Pb <sub>3</sub> , As <sub>3</sub> ClO <sub>12</sub> Sr <sub>5</sub> , As <sub>3</sub> ClO <sub>9</sub> Pb <sub>5</sub> , As <sub>3</sub> FO <sub>12</sub> Sr <sub>5</sub> , As <sub>6</sub> Cl <sub>2</sub> O <sub>18</sub> Pb <sub>10</sub> , As <sub>6</sub> Cl <sub>2</sub> O <sub>24</sub> Pb <sub>10</sub> , BB <sub>3</sub> , BCl <sub>3</sub> , BF <sub>3</sub> Mg <sub>3</sub> O <sub>3</sub> , Bi <sub>3</sub> , Ba <sub>3</sub> Nb <sub>2</sub> O <sub>9</sub> Sr, Ba <sub>3</sub> O <sub>9</sub> SrTa <sub>2</sub> , Ba <sub>4</sub> Nb <sub>2</sub> O <sub>9</sub> , Ba <sub>4</sub> O <sub>9</sub> Ta <sub>2</sub> , Bi <sub>2</sub> Ge <sub>3</sub> O <sub>9</sub> , Bi <sub>2</sub> O <sub>9</sub> Si <sub>3</sub> , Bi <sub>2</sub> S <sub>4</sub> Sr, Br <sub>2</sub> Sn, Br <sub>3</sub> La, Br <sub>3</sub> La <sub>9</sub> Sb <sub>16</sub> , Br <sub>9</sub> K <sub>3</sub> Mo <sub>2</sub> , CCl <sub>4</sub> NOSb, C <sub>3</sub> N <sub>4</sub> , CaMg <sub>2</sub> O <sub>12</sub> S <sub>3</sub> , Ca <sub>3</sub> Ge <sub>4</sub> , CdMo <sub>3</sub> O <sub>12</sub> Th, Cl <sub>18</sub> NNaW <sub>6</sub> , Cl <sub>3</sub> La, Cl <sub>3</sub> La <sub>3</sub> O <sub>6</sub> U, Cl <sub>3</sub> La <sub>3</sub> O <sub>6</sub> W, Cl <sub>9</sub> K <sub>3</sub> Mo <sub>2</sub> , Cl <sub>9</sub> K <sub>3</sub> W <sub>2</sub> , Cs <sub>2</sub> Ge <sub>3</sub> O <sub>9</sub> Sn, Cs <sub>2</sub> Ge <sub>3</sub> O <sub>9</sub> Ti, Cs <sub>2</sub> O <sub>9</sub> Si <sub>3</sub> Zr, Cs <sub>5</sub> Mo <sub>21</sub> S <sub>23</sub> , Cs <sub>5</sub> Mo <sub>21</sub> Se <sub>23</sub> , GaN <sub>3</sub> Sr <sub>3</sub> , Ga <sub>2</sub> O <sub>9</sub> Te <sub>3</sub> , Ge <sub>3</sub> N <sub>4</sub> , Ge <sub>3</sub> O <sub>9</sub> Sb <sub>2</sub> , Ge <sub>3</sub> O <sub>9</sub> TiTl <sub>2</sub> , Ge <sub>6</sub> Na <sub>4</sub> O <sub>15</sub> Sr, K <sub>2</sub> O <sub>9</sub> Si <sub>3</sub> Sn, K <sub>2</sub> O <sub>9</sub> Si <sub>3</sub> Ti, K <sub>2</sub> O <sub>9</sub> Si <sub>3</sub> Zr, K <sub>2</sub> O <sub>9</sub> Si <sub>4</sub> , Mo <sub>15</sub> S <sub>19</sub> , Mo <sub>9</sub> Se <sub>11</sub> , N <sub>4</sub> Si <sub>3</sub> , O <sub>9</sub> Rb <sub>2</sub> Si <sub>3</sub> Sn, O <sub>9</sub> Rb <sub>2</sub> Si <sub>3</sub> Th, O <sub>9</sub> Rb <sub>2</sub> Si <sub>3</sub> Ti, O <sub>9</sub> Sc <sub>2</sub> Se <sub>3</sub> ,
176	AgF <sub>3</sub> , AuF <sub>3</sub> ,
178	A <sub>11</sub> LiO <sub>4</sub> Si, BL <sub>a</sub> Pt <sub>2</sub> , C <sub>8</sub> Cs, CaO <sub>4</sub> S, Ge <sub>2</sub> Nb, HfSn <sub>2</sub> , Hg <sub>2</sub> INaO <sub>2</sub> , O <sub>2</sub> Si, Si <sub>2</sub> W,
180	A <sub>11</sub> LiO <sub>4</sub> Si, AlO <sub>4</sub> P,
181	Al <sub>2</sub> BaO <sub>4</sub> , BaHgO <sub>2</sub> , CaO <sub>11</sub> Ta <sub>4</sub> , F <sub>3</sub> La, IO <sub>6</sub> RbSn, O <sub>11</sub> SrTa <sub>4</sub> , O <sub>2</sub> Si, O <sub>3</sub> SbTl,
182	Ta <sub>21</sub> Te <sub>13</sub> ,
183	AsCs <sub>3</sub> , AsNa <sub>3</sub> , B <sub>3</sub> Ba <sub>3</sub> O <sub>9</sub> Sc, B <sub>9</sub> Li, Ba <sub>6</sub> Nb <sub>14</sub> O <sub>47</sub> Si <sub>4</sub> , Cs <sub>3</sub> F <sub>9</sub> Ga <sub>2</sub> , F <sub>3</sub> La, GaO <sub>3</sub> Y, GeLi <sub>8</sub> O <sub>6</sub> , I <sub>3</sub> RbTi, InO <sub>3</sub> Y, Li <sub>8</sub> O <sub>6</sub> Si, Lu <sub>2</sub> S <sub>3</sub> , NNa <sub>3</sub> , O <sub>3</sub> W, Pd <sub>5</sub> Sb <sub>2</sub> ,
184	AgGeLa, AlAs <sub>4</sub> Ca <sub>3</sub> Na <sub>3</sub> , AlCa <sub>3</sub> Na <sub>3</sub> Sb <sub>4</sub> , AlP, AlSb, Al <sub>4</sub> BeMgO <sub>8</sub> , AsBrHg <sub>3</sub> S <sub>4</sub> , AsBrHg <sub>3</sub> Se <sub>4</sub> , AsClHg <sub>3</sub> S <sub>4</sub> , AsHg <sub>3</sub> ISe <sub>4</sub> , As <sub>4</sub> GaNa <sub>3</sub> Sr <sub>3</sub> , BN, BP, BaN <sub>7</sub> Si <sub>4</sub> Y, Ba <sub>4</sub> Br <sub>6</sub> O, Ba <sub>4</sub> Cl <sub>6</sub> O, Ba <sub>4</sub> I <sub>6</sub> O, Ba <sub>4</sub> LiNb <sub>3</sub> O <sub>12</sub> , Ba <sub>4</sub> LiO <sub>12</sub> Ta <sub>3</sub> , Ba <sub>5</sub> Li <sub>2</sub> O <sub>15</sub> W <sub>3</sub> , BeO, Be <sub>4</sub> NaO <sub>7</sub> Sb, Bi <sub>2</sub> O <sub>3</sub> , Br <sub>2</sub> Cd, Br <sub>3</sub> CdCs, Br <sub>6</sub> OSr <sub>4</sub> , C, CSi, C <sub>3</sub> Al <sub>3</sub> Sc, C <sub>3</sub> Al <sub>5</sub> N, C <sub>4</sub> Al <sub>4</sub> Si, CaGe <sub>2</sub> , CaO, CaOSZn, Ca <sub>2</sub> O <sub>4</sub> Si, Ca <sub>4</sub> Cl <sub>6</sub> O, CdI <sub>2</sub> , CdK <sub>6</sub> O <sub>4</sub> , CdO, CdS, CdSe, CdTe, ClInK <sub>6</sub> Te <sub>4</sub> , Cl <sub>3</sub> La <sub>4</sub> NS <sub>3</sub> , Cl <sub>6</sub> OSr <sub>4</sub> , F <sub>8</sub> K <sub>3</sub> Ta, GaN, GaNa <sub>3</sub> P <sub>4</sub> Si <sub>3</sub> , GaP, GaSe, Ge <sub>8</sub> Li <sub>7</sub> Rb, HgK <sub>6</sub> S <sub>4</sub> , HgRb <sub>6</sub> S <sub>4</sub> , HgRb <sub>6</sub> Se <sub>4</sub> , ILi, I <sub>2</sub> Pb, I <sub>7</sub> Nb <sub>3</sub> Te, I <sub>7</sub> SeTa <sub>3</sub> , I <sub>7</sub> Ta <sub>3</sub> Te, InN, In <sub>2</sub> S <sub>4</sub> Zn, In <sub>2</sub> S <sub>5</sub> Zn <sub>2</sub> , KSbSn, K <sub>4</sub> O <sub>3</sub> Sb <sub>2</sub> , K <sub>6</sub> MgO <sub>4</sub> , LaMo <sub>2</sub> O <sub>5</sub> , LaN, LiMo <sub>2</sub> O <sub>8</sub> Tl <sub>3</sub> , LiSbZn, MgSe, MgTe, Mg <sub>2</sub> Mo <sub>3</sub> O <sub>8</sub> , Mo <sub>3</sub> O <sub>8</sub> Zn <sub>2</sub> , NTl, N <sub>7</sub> Si <sub>4</sub> SrY, NaPSn, Na <sub>6</sub> P <sub>4</sub> W, Na <sub>6</sub> S <sub>4</sub> Zn, O <sub>2</sub> Pt, O <sub>8</sub> SiSn <sub>6</sub> , P <sub>3</sub> Sc <sub>7</sub> , PdSnU, S <sub>2</sub> Sn, SeZn, Se <sub>2</sub> Ta, Si, TeZn,
185	AsBaLi, AsKZn, AuGaHf, AuGaZr, AuLuSi, AuScSi, BN, BaLiP, BrLi <sub>10</sub> N <sub>3</sub> , Br <sub>2</sub> Ca <sub>3</sub> Si, CHf, C <sub>2</sub> AgLi, GaSe, Ga <sub>4</sub> LiY, HfN <sub>2</sub> , Hg, InNbS <sub>2</sub> , InNbSe <sub>2</sub> , InS <sub>2</sub> Tl, InSe, KSbZn, LiPSr, LuPPt, NY, N <sub>2</sub> W, NbSe <sub>2</sub> , O <sub>2</sub> RbSc, PPtY, PbS,
186	BaGe <sub>3</sub> O <sub>9</sub> Sn, BaO <sub>9</sub> Si <sub>3</sub> Sn, BaO <sub>9</sub> Si <sub>3</sub> Ti, BaO <sub>9</sub> Si <sub>4</sub> , Be <sub>3</sub> F <sub>9</sub> KZn, BiO <sub>19</sub> Ta <sub>7</sub> , Ge <sub>3</sub> KO <sub>9</sub> Ta, Ge <sub>3</sub> NbO <sub>9</sub> Rb, Ge <sub>3</sub> O <sub>9</sub> RbTa, Ge <sub>3</sub> O <sub>9</sub> TaTl, LaO <sub>19</sub> Ta <sub>7</sub> ,
187	AgAsCa, AgCaP, AgGeSc, AgLaMg, AgLuSi, AgMgY, AgPbY, AgSiY, AlCsF <sub>4</sub> , AlMgY, AsCa, AsCs, AsLuPd, AsNaSr, AsSr, As <sub>2</sub> Sr <sub>2</sub> , AuCdLa, AuGaMg, Au <sub>2</sub> K <sub>38</sub> Na <sub>12</sub> Tl <sub>48</sub> , Au <sub>7</sub> IP <sub>10</sub> , BLiPt <sub>3</sub> , B <sub>2</sub> Ba <sub>3</sub> O <sub>12</sub> Ti <sub>3</sub> , BaBiNa, BaCl <sub>2</sub> , BaI <sub>2</sub> , BaNaP, Ba <sub>3</sub> Nb <sub>6</sub> O <sub>26</sub> Si <sub>4</sub> , Ba <sub>3</sub> O <sub>26</sub> Si <sub>4</sub> Ta <sub>6</sub> , Ba <sub>5</sub> Mg <sub>18</sub> Si <sub>13</sub> , CFMgO <sub>3</sub> Rb, CaCdGe, CaCdPb, CaCdSn, CaP, CaPbPd, Ca <sub>2</sub> P <sub>2</sub> , CsRb <sub>14</sub> Tl <sub>27</sub> , F <sub>6</sub> HfK <sub>2</sub> , F <sub>6</sub> K <sub>2</sub> Th, F <sub>6</sub> K <sub>2</sub> U, F <sub>6</sub> Rb <sub>2</sub> Th, GaLaMg, GaMgY, Ge <sub>12</sub> Mg <sub>19</sub> Sr <sub>5</sub> , GeLiY, GeO <sub>3</sub> Sr, GePdTl, Ge <sub>3</sub> La <sub>2</sub> Zn <sub>6</sub> , Ge <sub>4</sub> K <sub>6</sub> Nb <sub>6</sub> O <sub>26</sub> , InLaPt, InMgY, K <sub>2</sub> S <sub>2</sub> , K <sub>2</sub> Se <sub>2</sub> , K <sub>2</sub> Te <sub>2</sub> , K <sub>6</sub> O <sub>26</sub> Si <sub>4</sub> Ta <sub>6</sub> ,

Part 21 of all the predicted materials with band crossings from **Cases 1 or 2**:

189	<chem>LaMgTl</chem> , <chem>LiSiY</chem> , <chem>Lu6MoSb2</chem> , <chem>MgTiY</chem> , <chem>NaPSr</chem> , <chem>Na2O2</chem> , <chem>Na2S2</chem> , <chem>OTi</chem> , <chem>O26Si4Sr3Ta6</chem> , <chem>O2Ti</chem> , <chem>O8U3</chem> , <chem>PSr</chem> , <chem>Pd5Th3</chem> , <chem>PtSnU</chem> , <chem>Pt5Th3</chem> , <chem>Rb2S2</chem> , <chem>Rb2Se2</chem> , <chem>Rb2Te2</chem> , <chem>Se2U</chem> ,
190	<chem>Ag2Al2Bi2Cl8S3</chem> , <chem>Ag2I10Tl6</chem> , <chem>Ag5KS3</chem> , <chem>Ag5RbS3</chem> , <chem>Au6K4S5</chem> , <chem>Au6Rb4S5</chem> , <chem>CCl18W6</chem> , <chem>C3K3NaO11U</chem> , <chem>F3La3O9Si3</chem> , <chem>IO7Sb5</chem> , <chem>I2K9Li3O13</chem> , <chem>K3Nb3O13Si2</chem> ,
191	<chem>As4BrKO6</chem> , <chem>As4ClKO6</chem> , <chem>As4IKO6</chem> , <chem>B2Sr</chem> , <chem>B2Ti</chem> , <chem>B2Zr</chem> , <chem>BaSi2</chem> , <chem>BaSn5</chem> , <chem>C2Ca</chem> , <chem>CaPd5</chem> , <chem>CaSi2</chem> , <chem>CaZn5</chem> , <chem>FN3Ta2</chem> , <chem>Ga2Sr</chem> , <chem>Li2Pd</chem> , <chem>Li2Pt</chem> , <chem>Li3N</chem> , <chem>O144Si72</chem> , <chem>O3W</chem> , <chem>Pd5Sr</chem> , <chem>Si</chem> , <chem>Ti</chem> , <chem>Ti2Zr</chem> ,
193	<chem>As2O6Sr</chem> , <chem>Ca10Ge3Pt7</chem> , <chem>Ca10Pt7Si3</chem> , <chem>Ca6GaN5</chem> , <chem>GaN5Sr6</chem> , <chem>Ge3Ti5</chem> , <chem>Ge3Zr5</chem> , <chem>K2O3Pb</chem> , <chem>NbSb5U3</chem> , <chem>O19Ta6Th2</chem> , <chem>O2Si</chem> , <chem>O3W</chem> , <chem>Pb3SZr5</chem> , <chem>Pb3TeZr5</chem> , <chem>Pb3Zr5</chem> , <chem>Sn3Ti5</chem> , <chem>Sn3Zr5</chem> ,
194	<chem>AgAlO2</chem> , <chem>AgBaP</chem> , <chem>AgBaSb</chem> , <chem>AgGaO2</chem> , <chem>AgInO2</chem> , <chem>AgO2Sc</chem> , <chem>AgO2Y</chem> , <chem>AgPSr</chem> , <chem>AgSbSr</chem> , <chem>Al12O19Sr</chem> , <chem>AlAs</chem> , <chem>AlAuO2</chem> , <chem>AlBa2InO5</chem> , <chem>AlCs6K3Sb4</chem> , <chem>AlK6Na3Sb4</chem> , <chem>Alli</chem> , <chem>AlN</chem> , <chem>AlNTi2</chem> , <chem>AlNZr2</chem> , <chem>AlN3Nb4</chem> , <chem>AlN3Ti4</chem> , <chem>AlO3Y</chem> , <chem>Al22Na2O34</chem> , <chem>Al2Hf</chem> , <chem>Ar</chem> , <chem>AsBeNa</chem> , <chem>AsF5</chem> , <chem>AsHgK</chem> , <chem>AsKZn</chem> , <chem>AsK3</chem> , <chem>AsLi3</chem> , <chem>AsNa3</chem> , <chem>AsPtY</chem> , <chem>AsRb3</chem> , <chem>As2AuK5</chem> , <chem>AuBaBi</chem> , <chem>AuCs3O</chem> , <chem>AuGaO2</chem> , <chem>AuInO2</chem> , <chem>AuK5P2</chem> , <chem>AuO2Sc</chem> , <chem>AuO2Y</chem> , <chem>BMg3N3</chem> , <chem>BN</chem> , <chem>B2W</chem> , <chem>Ba</chem> , <chem>BaGaGe</chem> , <chem>BaLiP</chem> , <chem>BaLiSb</chem> , <chem>BaO</chem> , <chem>BaO3Si</chem> , <chem>BaO3Ti</chem> , <chem>BaS3Ti</chem> , <chem>BaSe3Ti</chem> , <chem>BaSe3Zr</chem> , <chem>Ba3BiN</chem> , <chem>Ba3NSb</chem> , <chem>Ba3Nb2O9Sr</chem> , <chem>Ba3O9SrTa2</chem> , <chem>Ba3O9Te2</chem> , <chem>Ba6O17Ti4Y2</chem> , <chem>Be</chem> , <chem>BeHfSi</chem> , <chem>BeNaSb</chem> , <chem>BeSe</chem> , <chem>BeSiZr</chem> , <chem>Be2Mo</chem> , <chem>Bi2Cs3I9</chem> , <chem>BrHg2N</chem> , <chem>BrK3Mo2O7</chem> , <chem>Br3CsMg</chem> , <chem>Br8Cs3Mo2</chem> , <chem>Br9Mo2Rb3</chem> , <chem>C</chem> , <chem>CBLi</chem> , <chem>CCdTi2</chem> , <chem>CGeNb2</chem> , <chem>CGeTi2</chem> , <chem>CHf2Pb</chem> , <chem>CHf2Sn</chem> , <chem>CK2O3</chem> , <chem>CN2O2Y2</chem> , <chem>CNa2O3</chem> , <chem>CNb2S</chem> , <chem>CNb2Sn</chem> , <chem>CPbTi2</chem> , <chem>CPbZr2</chem> , <chem>CSnTi2</chem> , <chem>CSnZr2</chem> , <chem>C2AlTa3</chem> , <chem>C2Al3O5Sc3</chem> , <chem>C2SiTi3</chem> , <chem>C2SnTi3</chem> , <chem>C3Al3Lu</chem> , <chem>C3Al3Sc</chem> , <chem>C3Al3Y</chem> , <chem>C6Au3Cs2N6Na</chem> , <chem>CaGaGe</chem> , <chem>CaGaSn</chem> , <chem>CaGa2P2</chem> , <chem>CaGeZn</chem> , <chem>CaIn2P2</chem> , <chem>CaSiZn</chem> , <chem>Ca2IN</chem> , <chem>Ca3N2</chem> , <chem>Ca4Mg13Zn29</chem> , <chem>Cd</chem> , <chem>CdCl3Cs</chem> , <chem>CdMg3</chem> , <chem>CdNa2Sn</chem> , <chem>Cl3CsMg</chem> , <chem>Cl3MgRb</chem> , <chem>Cl5Sb</chem> , <chem>Cl9Cs3Mo2</chem> , <chem>Cl9Cs3Ti2</chem> , <chem>Cl9Cs3W2</chem> , <chem>Cl9Mo2Rb3</chem> , <chem>Cs</chem> , <chem>CsI3Mg</chem> , <chem>CsLuS2</chem> , <chem>Cs2O4S</chem> , <chem>Cs2Pt</chem> , <chem>Cs3F3Mo2O6</chem> , <chem>Cs3I9Mo2</chem> , <chem>Cs3I9Sb2</chem> , <chem>Cs3I9Y2</chem> , <chem>Cs3I9Zr2</chem> , <chem>Cs6GaK3Sb4</chem> , <chem>F18Mg6Rb6</chem> , <chem>FSY</chem> , <chem>F2Sr</chem> , <chem>F3La</chem> , <chem>F3MgRb</chem> , <chem>F3RbZn</chem> , <chem>GaGeSr</chem> , <chem>GaInO3</chem> , <chem>GaInO5Zn2</chem> , <chem>GaInO7Zn4</chem> , <chem>GaK6Na3Sb4</chem> , <chem>GaS</chem> , <chem>GaSe</chem> , <chem>GaSnSr</chem> , <chem>GaTe</chem> , <chem>He</chem> , <chem>HfN2</chem> , <chem>HfP</chem> , <chem>Hf9Re4S</chem> , <chem>Hf9Re4Se</chem> , <chem>HgKSB</chem> , <chem>Hg3U</chem> , <chem>ILa</chem> , <chem>ILi</chem> , <chem>IORb3</chem> , <chem>I2K4O9</chem> , <chem>I2Th</chem> , <chem>InNTi2</chem> , <chem>InNZr2</chem> , <chem>InPt2Y</chem> , <chem>InS2Ta</chem> , <chem>InS2Tl</chem> , <chem>InSe</chem> , <chem>In2P2Sr</chem> , <chem>KNbS2</chem> , <chem>KNbSe2</chem> , <chem>KPZn</chem> , <chem>KSbZn</chem> , <chem>KTL</chem> , <chem>K2O4S</chem> , <chem>K2Te2</chem> , <chem>K3LaO9Te2</chem> , <chem>K3LuO7Si2</chem> , <chem>K3O7ScSi2</chem> , <chem>K3P</chem> , <chem>K3Sb</chem> , <chem>Kr</chem> , <chem>LiNbO2</chem> , <chem>LiNbS2</chem> , <chem>LiPSr</chem> , <chem>Li2O2</chem> , <chem>Li3N</chem> , <chem>Li3P</chem> , <chem>Li3Sb</chem> , <chem>LuMg2</chem> , <chem>Mg</chem> , <chem>Mg17Sr2</chem> , <chem>MgMoN2</chem> , <chem>MgO</chem> , <chem>MgPo</chem> , <chem>MgTe</chem> , <chem>Mg4Sr</chem> , <chem>MoS2</chem> , <chem>MoSe2</chem> , <chem>MoTe2</chem> , <chem>NY</chem> , <chem>N2SZr2</chem> , <chem>N2SeZr2</chem> , <chem>N2W</chem> , <chem>Na13Pb5</chem> , <chem>NaNbO2</chem> , <chem>NaNbS2</chem> , <chem>NaNbSe2</chem> , <chem>NaS</chem> , <chem>Na2O4S</chem> , <chem>Na2S2</chem> , <chem>Na2Se2</chem> , <chem>Na3P</chem> , <chem>Na3Sb</chem> , <chem>O2RbSc</chem> , <chem>O2SSc2</chem> , <chem>O2Si</chem> , <chem>O4Rb2S</chem> , <chem>O4STl2</chem> , <chem>PbPt</chem> , <chem>PbS</chem> , <chem>PdSnU</chem> , <chem>PoZr</chem> , <chem>PtSn</chem> , <chem>Pt2SnU</chem> , <chem>RbTe2Y</chem> , <chem>Rb2S</chem> , <chem>Rb2Te</chem> , <chem>Rb3Sb</chem> , <chem>Re2Y</chem> , <chem>S2ScTl</chem> , <chem>S2Ti</chem> , <chem>S2W</chem> , <chem>ScZn2</chem> , <chem>Se2W</chem> , <chem>SiSrZn</chem> , <chem>SiSr2</chem> , <chem>SnTi2</chem> , <chem>SnTi3</chem> , <chem>TaZn2</chem> , <chem>Te2W</chem> , <chem>Xe</chem> , <chem>Zn</chem> ,

Part 22 of all the predicted materials with band crossings from **Cases 1 or 2:**

195	<chem>I4Sn</chem> , <chem>O2Si</chem> ,
196	<chem>Ge5Li22</chem> , <chem>Li22Pb5</chem> , <chem>Li22Sn5</chem> ,
197	<chem>Al6Ca4O16S</chem> , <chem>Al6O16SSr4</chem> , <chem>Al6O16Sr4W</chem> , <chem>Bi12GeO20</chem> , <chem>Bi12O20Si</chem> , <chem>Bi12O20Ti</chem> , <chem>Bi24O40Pb2</chem> , <chem>Bi24O40Si2</chem> , <chem>Bi24O40Ti2</chem> , <chem>Bi2O3</chem> , <chem>Cs18O6Tl8</chem> , <chem>Li3NbO4</chem> ,
198	<chem>Ag3NO3S</chem> , <chem>Ag7AsS6</chem> , <chem>Ag7AsSe6</chem> , <chem>Ag7PS6</chem> , <chem>AlNaO4Si</chem> , <chem>Al2Ba3O6</chem> , <chem>AsClHg3O4</chem> , <chem>AsK3S3</chem> , <chem>AsK3Se3</chem> , <chem>AsNa3S3</chem> , <chem>AsNa3Se3</chem> , <chem>As4Br6Hg6Sn</chem> , <chem>BKMgO3</chem> , <chem>BMgO3Rb</chem> , <chem>BaN2O6</chem> , <chem>Be3Cd2F12Rb2</chem> , <chem>BiCs3O3</chem> , <chem>BiCs3Se3</chem> , <chem>BiK2RbSe3</chem> , <chem>BiK3Se3</chem> , <chem>BiK3Te3</chem> , <chem>BiO3Rb3</chem> , <chem>BiRb3Se3</chem> , <chem>BrNaO3</chem> , <chem>BrP7Sr2</chem> , <chem>Br6Hg7P4Sn</chem> , <chem>CaNa2O4Si</chem> , <chem>ClF3Sn2</chem> , <chem>ClIn</chem> , <chem>ClNaO3</chem> , <chem>Cl4Hg3O</chem> , <chem>Cl6Hg6P4Pb</chem> , <chem>CsF7Xe</chem> , <chem>Cs2Mg2O12W3</chem> , <chem>Cs3O3Sb</chem> , <chem>Cs3S3Sb</chem> , <chem>Cs3SbSe3</chem> , <chem>F4LiSb</chem> , <chem>HfOS</chem> , <chem>HfO8W2</chem> , <chem>HgPd</chem> , <chem>IP7Sr2</chem> , <chem>K2Mg2O12S3</chem> , <chem>K2O12S3Zn2</chem> , <chem>K3O3Sb</chem> , <chem>K3S3Sb</chem> , <chem>K3SbSe3</chem> , <chem>K3SbTe3</chem> , <chem>MgPt</chem> , <chem>Mg2Mo3O12Tl2</chem> , <chem>Mg2O12Rb2W3</chem> , <chem>MoNa2O6Se</chem> , <chem>N11Na3P6</chem> , <chem>N2</chem> , <chem>Na3S3Sb</chem> , <chem>Na3SbSe3</chem> , <chem>Na3SbTe3</chem> , <chem>OSZr</chem> , <chem>O2Si</chem> , <chem>O3SrZr</chem> , <chem>O4SnW</chem> , <chem>O8W2Zr</chem> , <chem>P2Pb3S8</chem> , <chem>Rb3S3Sb</chem> , <chem>Rb3SbSe3</chem> , <chem>SbSe3Tl3</chem> , <chem>Te3Tl2Zr</chem> ,
199	<chem>Al2Ca3F14Na2</chem> , <chem>Br2Hg3Te2</chem> , <chem>Cl2Hg3S2</chem> , <chem>Cl2Hg3Se2</chem> , <chem>Cl2Hg3Te2</chem> , <chem>F2Hg3S2</chem> , <chem>In2O3</chem> , <chem>K2O3Pb2</chem> , <chem>K2O3Sn2</chem> , <chem>Lu2O3</chem> , <chem>N</chem> , <chem>O2Si</chem> , <chem>O3Sc2</chem> , <chem>O3Tl2</chem> , <chem>O3Y2</chem> , <chem>Pb2Pd3S2</chem> ,
200	<chem>AsBr3Ca3</chem> , <chem>CaO6Ta2</chem> , <chem>Cd11Na2</chem> , <chem>Cl7Na</chem> , <chem>K6MgNa14Tl18</chem> , <chem>K6Na14Tl18Zn</chem> , <chem>LuNaO8Pd6</chem> , <chem>Mg2Zn11</chem> ,
201	<chem>BiKO3</chem> , <chem>Br14CdW6</chem> , <chem>Br14Mo6Pb</chem> , <chem>C2Ca</chem> , <chem>KO3Sb</chem> ,
203	<chem>AsRb3Se16</chem> , <chem>O2Si</chem> ,
204	<chem>Al12Mo</chem> , <chem>Al12W</chem> , <chem>BaGe12Pt4</chem> , <chem>C10Cs</chem> , <chem>C8</chem> , <chem>CaO12Pd3Ti4</chem> , <chem>CaO3Si</chem> , <chem>NPd3</chem> , <chem>N2O4</chem> ,
205	<chem>AgPd3Se</chem> , <chem>Ag2As4Hg7I6</chem> , <chem>AlF6K2Na</chem> , <chem>As2Br3Cd4</chem> , <chem>As2Br3Hg4</chem> , <chem>As2Pd</chem> , <chem>As2Pt</chem> , <chem>As4BiCl7Hg6</chem> , <chem>As4Br7Hg6In</chem> , <chem>As4Cl7Hg6In</chem> , <chem>As4Cl7Hg6Mo</chem> , <chem>Au3CaGa</chem> , <chem>Au3GeNa</chem> , <chem>Au3NaSi</chem> , <chem>BaF7Ta</chem> , <chem>BaGa2S4</chem> , <chem>Br7Hg6InSb4</chem> , <chem>Br7Hg6Sb5</chem> , <chem>Br9In7</chem> , <chem>CO2</chem> , <chem>C2Si</chem> , <chem>C60</chem> , <chem>CdO2</chem> , <chem>CdS2</chem> , <chem>CdSe2</chem> , <chem>Cd7Cl6P4</chem> , <chem>Cl12I2Nb6</chem> , <chem>Cl9In7</chem> , <chem>CsF7W</chem> , <chem>CsO6Se2Y</chem> , <chem>F2Mg</chem> , <chem>F6NaSb</chem> , <chem>Ga4GeS4</chem> , <chem>GeI4</chem> , <chem>GeO2</chem> , <chem>GeO6Se2</chem> , <chem>Ge8NaRb7</chem> , <chem>HfN2</chem> , <chem>I4Sn</chem> , <chem>In4S4Sn</chem> , <chem>K7LiSi3</chem> , <chem>Li7N4Nb</chem> , <chem>MgO2</chem> , <chem>MgSe2</chem> , <chem>MgTe2</chem> , <chem>N2</chem> , <chem>N2Pd</chem> , <chem>N2Pt</chem> , <chem>N2W</chem> , <chem>NaRb7Si8</chem> , <chem>O2Pt</chem> , <chem>O2Sn</chem> , <chem>O2Sn</chem> , <chem>O2U</chem> , <chem>O6Se2Sn</chem> , <chem>O7P2Si</chem> , <chem>P2Pt</chem> , <chem>P2Si</chem> , <chem>PdSb2</chem> , <chem>PtSb2</chem> , <chem>S2Ti</chem> , <chem>S2Zn</chem> , <chem>Se2Zn</chem> ,
206	<chem>AgF6Sb</chem> , <chem>AlLi3N2</chem> , <chem>As2Mg3</chem> , <chem>Be3N2</chem> , <chem>Be3P2</chem> , <chem>BiF6K</chem> , <chem>Bi2O3</chem> , <chem>C</chem> , <chem>Ca3N2</chem> , <chem>Cd3N2</chem> , <chem>Cd3P2</chem> , <chem>F6KSb</chem> , <chem>Gal3N2</chem> , <chem>HfO8Te3</chem> , <chem>In2O3</chem> , <chem>La2O3</chem> , <chem>Li3N2Sc</chem> , <chem>Lu2O3</chem> , <chem>Mg3N2</chem> , <chem>Mg3P2</chem> , <chem>Mg3Sb2</chem> , <chem>N2Zn3</chem> , <chem>O2Si</chem> , <chem>O3Sc2</chem> , <chem>O3Tl2</chem> , <chem>O3Y2</chem> , <chem>O8SnTe3</chem> , <chem>O8Te3Ti</chem> , <chem>O8Te3Zr</chem> , <chem>P2Zn3</chem> ,
212	<chem>Bi2K3N9O27</chem> , <chem>O8Ti3Zn2</chem> ,
213	<chem>Ag4S8Sn3</chem> , <chem>Be2CsF5</chem> , <chem>CAI2Mo3</chem> , <chem>Cs3N11P6</chem> , <chem>K3N11P6</chem> , <chem>N11P6Rb3</chem> , <chem>Si2Sr</chem> ,
214	<chem>Ag3AuSe2</chem> , <chem>Ag3AuTe2</chem> , <chem>AsI3La3</chem> , <chem>BBa2ClN2</chem> , <chem>Ca3I3P</chem> , <chem>Ca3O12Te2Zn3</chem> , <chem>I3La3P</chem> , <chem>I3La3Sb</chem> ,
215	<chem>Au9In4</chem> , <chem>Be4Na10O17Si4</chem> , <chem>BiF3</chem> , <chem>BiMg63Si32</chem> , <chem>CCs4O4</chem> , <chem>CK4O4</chem> , <chem>CLi4O4</chem> , <chem>CNa4O4</chem> , <chem>C2N2Zn</chem> , <chem>C3N2</chem> , <chem>C3N4</chem> , <chem>C4BLiN4</chem> , <chem>In5Tl8</chem> , <chem>Li2MgSi</chem> ,

Part 23 of all the predicted materials with band crossings from **Cases 1 or 2:**

216	AgI, AgKO, AgN, AgNaO, AgORb, AlAs, AlBB <sub>e</sub> , AlGeLi, AlLiSi, AlN, AlP, AlSb, Al <sub>4</sub> La <sub>17</sub> N <sub>33</sub> Si <sub>9</sub> , AsB, AsGa, AsLiMg, AsLiZn, Au <sub>10</sub> Mo <sub>4</sub> Zn <sub>89</sub> , AuGaLi <sub>2</sub> , AuLi <sub>2</sub> Tl, AuLuSn, AuScSn, B <sub>11</sub> Li, BN, BP, BSb, BaO <sub>4</sub> S, Ba <sub>3</sub> In <sub>2</sub> O <sub>11</sub> Zn <sub>5</sub> , Ba <sub>3</sub> Lu <sub>2</sub> O <sub>11</sub> Zn <sub>5</sub> , Be <sub>17</sub> Ca <sub>12</sub> O <sub>29</sub> , BeO, BePo, BeS, BeTe, Be <sub>4</sub> O <sub>7</sub> Te, Be <sub>5</sub> Pd, Be <sub>5</sub> Pt, BrMoS, C, CGe, CHf, CPt, CSi, CSn, CZr, Ca <sub>16</sub> N <sub>34</sub> Si <sub>17</sub> , CaSe, CdLiP, CdS, CdSe, CdTe, Cd <sub>45</sub> Y <sub>11</sub> , ClCsO <sub>4</sub> , ClKO <sub>4</sub> , ClNaO <sub>4</sub> , ClO <sub>4</sub> Rb, ClO <sub>4</sub> Tl, CsLiMoO <sub>4</sub> , GaLiSi, GaN, GaP, GeLi <sub>2</sub> Sn, GeLi <sub>2</sub> Zn, GePtTi, GeTi <sub>2</sub> , HfPdSn, HfPtSn, HgS, Hg <sub>45</sub> U <sub>11</sub> , InLaPt <sub>4</sub> , InN, InP, K <sub>3</sub> Sb, LiMgP, LiNZn, LiPZn, Li <sub>21</sub> Si <sub>5</sub> , MgS, MgSe, MgTe, NRe, NSc, NTa, NTI, NY, OZn, O <sub>4</sub> SSr, O <sub>4</sub> SZn, PSc, Pd <sub>17</sub> Te <sub>4</sub> , PdSbSc, PdSnZr, Pd <sub>4</sub> Te, PtSbSc, PtSbY, PtSnTh, PtSnTi, PtSnU, Pt <sub>5</sub> U, Re <sub>4</sub> S <sub>4</sub> Te <sub>4</sub> , SSn, SZn, SeZn, Si, SiSn, SnTe, SnTi <sub>2</sub> , TeZn,
217	Ag <sub>3</sub> Ge <sub>3</sub> P <sub>6</sub> Sn <sub>2</sub> , Ag <sub>3</sub> P <sub>6</sub> Si <sub>3</sub> Sn <sub>2</sub> , Al <sub>12</sub> Ca <sub>8</sub> O <sub>24</sub> S <sub>2</sub> , Al <sub>12</sub> Ca <sub>8</sub> O <sub>24</sub> Te <sub>2</sub> , Al <sub>12</sub> Cd <sub>8</sub> O <sub>24</sub> S <sub>2</sub> , Al <sub>12</sub> Cd <sub>8</sub> O <sub>24</sub> Te <sub>2</sub> , Al <sub>12</sub> O <sub>24</sub> S <sub>2</sub> Sn <sub>8</sub> , Al <sub>12</sub> O <sub>24</sub> Sn <sub>8</sub> Te <sub>2</sub> , Al <sub>6</sub> Ca <sub>4</sub> O <sub>13</sub> , Al <sub>6</sub> Ca <sub>4</sub> O <sub>16</sub> W, B <sub>12</sub> O <sub>24</sub> Se <sub>2</sub> Zn <sub>8</sub> , BiK <sub>3</sub> O <sub>3</sub> , BiNa <sub>3</sub> O <sub>3</sub> , CaNa <sub>10</sub> Sn <sub>12</sub> , Cd <sub>4</sub> N <sub>12</sub> P <sub>6</sub> S, F <sub>4</sub> Ge, F <sub>4</sub> Si, K <sub>3</sub> S <sub>4</sub> Sb, Li <sub>3</sub> NbO <sub>4</sub> , Mg <sub>4</sub> N <sub>12</sub> P <sub>6</sub> S, N <sub>12</sub> P <sub>6</sub> Sn <sub>4</sub> , N <sub>2</sub> , N <sub>24</sub> O <sub>2</sub> P <sub>12</sub> Zn <sub>8</sub> , Na <sub>10</sub> Sn <sub>12</sub> Sr, Na <sub>3</sub> O <sub>3</sub> Sb, Na <sub>3</sub> PSe <sub>4</sub> , Na <sub>3</sub> S <sub>4</sub> Sb, Na <sub>3</sub> SbSe <sub>4</sub> , NbS <sub>4</sub> Tl <sub>3</sub> , NbSe <sub>4</sub> Tl <sub>3</sub> , Nb <sub>3</sub> Sb <sub>2</sub> Te <sub>5</sub> , O <sub>2</sub> Si, S <sub>4</sub> TaTl <sub>3</sub> , Se <sub>4</sub> TaTl <sub>3</sub> , Si,
218	Ag <sub>3</sub> AsO <sub>4</sub> , Al <sub>6</sub> Br <sub>2</sub> Ge <sub>6</sub> Li <sub>8</sub> O <sub>24</sub> , Al <sub>6</sub> Br <sub>2</sub> Ge <sub>6</sub> Na <sub>8</sub> O <sub>24</sub> , Al <sub>6</sub> Cl <sub>2</sub> Ge <sub>6</sub> Na <sub>8</sub> O <sub>24</sub> , Al <sub>6</sub> Cl <sub>2</sub> K <sub>8</sub> O <sub>24</sub> Si <sub>6</sub> , Al <sub>6</sub> Cl <sub>2</sub> Na <sub>8</sub> O <sub>24</sub> Si <sub>6</sub> , Al <sub>6</sub> Ge <sub>6</sub> I <sub>2</sub> Li <sub>8</sub> O <sub>24</sub> , Al <sub>6</sub> Ge <sub>6</sub> I <sub>2</sub> Na <sub>8</sub> O <sub>24</sub> , Al <sub>6</sub> I <sub>2</sub> Na <sub>8</sub> O <sub>24</sub> Si <sub>6</sub> , As <sub>3</sub> Be <sub>3</sub> Cl <sub>11</sub> iO <sub>12</sub> , As <sub>4</sub> Ba <sub>4</sub> Ge, As <sub>4</sub> Ba <sub>4</sub> Si, As <sub>4</sub> Ba <sub>4</sub> Ti, As <sub>4</sub> Sr <sub>4</sub> Ti, As <sub>8</sub> Ge <sub>38</sub> I <sub>8</sub> , Ba <sub>4</sub> P <sub>4</sub> Si, BeCl <sub>2</sub> , BeF <sub>2</sub> , Be <sub>6</sub> Cd <sub>8</sub> O <sub>24</sub> S <sub>2</sub> Si <sub>6</sub> , Be <sub>6</sub> Cd <sub>8</sub> O <sub>24</sub> Se <sub>2</sub> Si <sub>6</sub> , Be <sub>6</sub> O <sub>24</sub> S <sub>2</sub> Si <sub>6</sub> Zn <sub>8</sub> , Br <sub>2</sub> Ga <sub>6</sub> Li <sub>8</sub> O <sub>24</sub> Si <sub>6</sub> , Br <sub>2</sub> Ga <sub>6</sub> Na <sub>8</sub> O <sub>24</sub> Si <sub>6</sub> , Br <sub>8</sub> Ge <sub>38</sub> P <sub>8</sub> , Cl <sub>2</sub> Ga <sub>6</sub> Li <sub>8</sub> O <sub>24</sub> Si <sub>6</sub> , Cl <sub>4</sub> Se, CsSi, Cs <sub>4</sub> Ge <sub>4</sub> , Cs <sub>4</sub> Se <sub>4</sub> Si, Cs <sub>8</sub> Sn <sub>8</sub> , Ga <sub>6</sub> I <sub>2</sub> Li <sub>8</sub> O <sub>24</sub> Si <sub>6</sub> , GeK, GeK <sub>4</sub> Se <sub>4</sub> , GeRb, Ge <sub>38</sub> I <sub>8</sub> P <sub>8</sub> , Ge <sub>4</sub> K <sub>4</sub> , Ge <sub>4</sub> Rb <sub>4</sub> , KSi, K <sub>4</sub> Si <sub>4</sub> , P <sub>4</sub> S <sub>4</sub> Ti, RbSi, Rb <sub>4</sub> S <sub>4</sub> Sn, Rb <sub>4</sub> Si <sub>4</sub> ,
219	Cl <sub>16</sub> Ge <sub>6</sub> , Cl <sub>16</sub> Si <sub>6</sub> ,
220	Ag <sub>3</sub> F <sub>24</sub> Sb <sub>4</sub> , Al <sub>14</sub> Ca <sub>12</sub> O <sub>32</sub> , AlO <sub>9</sub> P <sub>3</sub> , Au <sub>3</sub> La <sub>3</sub> Sb <sub>4</sub> , Bi <sub>4</sub> Ge <sub>3</sub> O <sub>12</sub> , Bi <sub>4</sub> O <sub>12</sub> Si <sub>3</sub> , C <sub>8</sub> Ag <sub>4</sub> Cs <sub>5</sub> IN <sub>8</sub> , Ca <sub>12</sub> Li <sub>6</sub> Mo <sub>4</sub> N <sub>16</sub> O <sub>3</sub> ,
221	AgF <sub>3</sub> Zn, AgGa, AgI, AgIn, AgLi, AgNbO <sub>3</sub> , AlAu, AlBiO <sub>3</sub> , AlF <sub>3</sub> , AlLaO <sub>3</sub> , AlSc, AlY, AsCa <sub>3</sub> Cl <sub>3</sub> , AsCa <sub>3</sub> N, AuCs, B <sub>6</sub> Ba, B <sub>6</sub> Ca, B <sub>6</sub> Si, B <sub>6</sub> Sr, BaF <sub>3</sub> Li, BaO <sub>3</sub> Sn, BaO <sub>3</sub> Ti, BaO <sub>3</sub> Zr, BaSe, BaTe, BeCsF <sub>3</sub> , BeTi, BiCa <sub>3</sub> N, BiGaO <sub>3</sub> , BiInO <sub>3</sub> , BiK <sub>9</sub> O <sub>24</sub> U <sub>6</sub> , BiNSr <sub>3</sub> , BiO <sub>3</sub> Sc, BrCs, BrK, BrLi <sub>3</sub> O, BrRb, BrTl, Br <sub>3</sub> CaCs, Br <sub>3</sub> CdCs, Br <sub>3</sub> CsGe, Br <sub>3</sub> CsPb, CPbPd <sub>3</sub> , CPt <sub>3</sub> Sn, CTh, C <sub>3</sub> N <sub>2</sub> , C <sub>3</sub> Nb <sub>4</sub> , CaCsF <sub>3</sub> , CaF <sub>3</sub> Li, CaF <sub>3</sub> Rb, CaO <sub>3</sub> Si, CaO <sub>3</sub> Sn, CaO <sub>3</sub> Ti, CaPd, Ca <sub>3</sub> Cl <sub>3</sub> P, Ca <sub>3</sub> GeO, Ca <sub>3</sub> NP, Ca <sub>3</sub> OPb, Ca <sub>3</sub> OSn, CdCl <sub>3</sub> Cs, CdCsF <sub>3</sub> , CdF <sub>3</sub> K, CdF <sub>3</sub> Rb, ClCs, ClK, ClNa, ClNa <sub>3</sub> O, ClRb, ClTl, Cl <sub>3</sub> CsHg, Cl <sub>3</sub> CsPb, Cl <sub>3</sub> CsSn, CsF <sub>3</sub> Hg, CsF <sub>3</sub> Pb, CsF <sub>3</sub> Sr, CsI, CsI <sub>3</sub> Pb, CsI <sub>3</sub> Sn, F <sub>3</sub> HgRb, F <sub>3</sub> KMg, F <sub>3</sub> KZn, F <sub>3</sub> MgNa, F <sub>3</sub> MgRb, F <sub>3</sub> Mg <sub>3</sub> N, F <sub>3</sub> Sc, F <sub>3</sub> Y, GeI <sub>3</sub> Rb, GeO <sub>3</sub> Pb, GeO <sub>3</sub> Sr, HfO <sub>3</sub> Pb, HfO <sub>3</sub> Sr, HfPd <sub>3</sub> , HgMg, HgPt <sub>3</sub> , HgTi <sub>3</sub> , IK, IRb, ITl, KNbO <sub>3</sub> , KO <sub>3</sub> Ta, LaN, LiTl, Li <sub>9</sub> NS <sub>3</sub> , MgO, MgPd, NSbSr <sub>3</sub> , NTi <sub>3</sub> Tl, NY, N <sub>3</sub> TaTh, NaNbO <sub>3</sub> , NaO <sub>3</sub> Ta, OSnSr <sub>3</sub> , OSr, OZn, O <sub>3</sub> PbTi, O <sub>3</sub> PbZr, O <sub>3</sub> SiSr, O <sub>3</sub> SnSr, O <sub>3</sub> SnTi, O <sub>3</sub> SrTi, O <sub>3</sub> SrZr,

Part 24 of all the predicted materials with band crossings from **Cases 1 or 2**:

221	O <sub>3</sub> U, O <sub>3</sub> W, PbPt <sub>3</sub> , PbS, PbSe, PbTe, Pt <sub>3</sub> Sn, Pt <sub>3</sub> Zn, SSr, SiU <sub>3</sub> , SnTe, Sn <sub>3</sub> U,
223	BiNb <sub>3</sub> , C <sub>60</sub> Ba <sub>3</sub> , Cl <sub>2</sub> Hg <sub>3</sub> S <sub>2</sub> , HgTi <sub>3</sub> , HgZr <sub>3</sub> , MgO, Nb <sub>3</sub> Sb, SbTa <sub>3</sub> , SbTa <sub>3</sub> , Si, Si <sub>46</sub> ,
224	Al <sub>2</sub> LuO <sub>8</sub> Pb <sub>2</sub> , Au <sub>2</sub> S, C <sub>2</sub> N <sub>4</sub> Si, Mg <sub>3</sub> P <sub>2</sub> , O <sub>2</sub> Si,
225	AgBr, AgCl, AgI, Ag <sub>2</sub> MgZn, Al <sub>16</sub> Pt <sub>7</sub> Zr <sub>6</sub> , AlAu <sub>2</sub> Sc, AlF <sub>6</sub> K <sub>2</sub> Li, AlF <sub>6</sub> K <sub>2</sub> Na, AlF <sub>6</sub> K <sub>3</sub> , AlF <sub>6</sub> NaRb <sub>2</sub> , AlN, Al <sub>2</sub> O, Al <sub>4</sub> In <sub>3</sub> Sr <sub>11</sub> , AsF <sub>6</sub> Na, AsLu, AsNa <sub>3</sub> , AsSc, AsY, AuLi <sub>3</sub> , Au <sub>2</sub> Cl <sub>6</sub> Cs <sub>2</sub> , Au <sub>2</sub> InLu, Au <sub>2</sub> InSc, Au <sub>2</sub> InY, B <sub>12</sub> Hf, B <sub>12</sub> Th, Ba, BaBiO <sub>3</sub> , BaO, BaPo, BaS, BaSe, BaTe, Ba <sub>2</sub> Bi <sub>2</sub> O <sub>6</sub> , Ba <sub>2</sub> CaMoO <sub>6</sub> , Ba <sub>2</sub> CaO <sub>6</sub> Te, Ba <sub>2</sub> CaO <sub>6</sub> W, Ba <sub>2</sub> CdO <sub>6</sub> U, Ba <sub>2</sub> INaO <sub>6</sub> , Ba <sub>2</sub> InNbO <sub>6</sub> , Ba <sub>2</sub> InO <sub>6</sub> Ta, Ba <sub>2</sub> LiO <sub>6</sub> Re, Ba <sub>2</sub> LuNbO <sub>6</sub> , Ba <sub>2</sub> LuO <sub>6</sub> Sb, Ba <sub>2</sub> LuO <sub>6</sub> Ta, Ba <sub>2</sub> MgO <sub>6</sub> Te, Ba <sub>2</sub> MgO <sub>6</sub> U, Ba <sub>2</sub> MgO <sub>6</sub> W, Ba <sub>2</sub> NaO <sub>6</sub> Re, Ba <sub>2</sub> NbO <sub>6</sub> Y, Ba <sub>2</sub> O <sub>6</sub> PbU, Ba <sub>2</sub> O <sub>6</sub> SbY, Ba <sub>2</sub> O <sub>6</sub> SrU, Ba <sub>2</sub> O <sub>6</sub> TaY, Ba <sub>2</sub> O <sub>6</sub> TeZn, Ba <sub>2</sub> O <sub>6</sub> UZn, Ba <sub>2</sub> O <sub>6</sub> WZn, Ba <sub>3</sub> O <sub>6</sub> W, BeO, BeSe, BiCl <sub>6</sub> Cs <sub>2</sub> Na, BiCs <sub>2</sub> F <sub>6</sub> K, BiCs <sub>2</sub> F <sub>6</sub> Na, BiCs <sub>2</sub> F <sub>6</sub> Rb, BiCs <sub>3</sub> , BiF <sub>3</sub> , BiF <sub>6</sub> KRb <sub>2</sub> , BiF <sub>6</sub> NaRb <sub>2</sub> , BiI <sub>3</sub> , BiLa, BiLi <sub>3</sub> , BiLu, BiRb <sub>3</sub> , BiSc, BiY, BrCs, BrK, BrLi, BrNa, BrRb, BrTl, Br <sub>6</sub> Cs <sub>2</sub> LaNa, Br <sub>6</sub> Cs <sub>2</sub> NaY, Br <sub>6</sub> Cs <sub>2</sub> Po, Br <sub>6</sub> Cs <sub>2</sub> Pt, Br <sub>6</sub> Cs <sub>2</sub> Sn, Br <sub>6</sub> Cs <sub>2</sub> Te, Br <sub>6</sub> Cs <sub>2</sub> U, Br <sub>6</sub> K <sub>2</sub> Pt, Br <sub>6</sub> K <sub>2</sub> Se, Br <sub>6</sub> K <sub>2</sub> Sn, Br <sub>6</sub> K <sub>2</sub> Te, Br <sub>6</sub> PdRb <sub>2</sub> , Br <sub>6</sub> Rb <sub>2</sub> Sn, Br <sub>6</sub> Rb <sub>2</sub> Te, Br <sub>6</sub> Rb <sub>2</sub> U, Br <sub>8</sub> Li <sub>6</sub> Mg, CBe <sub>2</sub> , CGe, CPd, CPt, CSi, CSn, CW, CZr, Ca, Ca <sub>11</sub> Ga <sub>7</sub> , CaF <sub>2</sub> , CaF <sub>6</sub> Pb, CaF <sub>6</sub> Sn, CaMoO <sub>6</sub> Sr <sub>2</sub> , CaO, CaO <sub>3</sub> Sn, CaO <sub>6</sub> Sr <sub>2</sub> W, CaPo, CaS, CaSe, CaTe, Ca <sub>2</sub> Ge, Ca <sub>2</sub> O <sub>6</sub> SiTi, Ca <sub>2</sub> Pb, Ca <sub>2</sub> Si, Ca <sub>2</sub> Sn, Ca <sub>3</sub> CdsPt <sub>4</sub> , Ca <sub>7</sub> Ge, CdCl <sub>8</sub> Na <sub>6</sub> , CdF <sub>2</sub> , CdO, CdO <sub>6</sub> Sr <sub>2</sub> W, CdS, CdSe, CdTe, ClCs, ClK, ClNa, ClRb, ClTl, Cl <sub>2</sub> Sr, Cl <sub>6</sub> Cs <sub>2</sub> Ge, Cl <sub>6</sub> Cs <sub>2</sub> KSc, Cl <sub>6</sub> Cs <sub>2</sub> LiLu, Cl <sub>6</sub> Cs <sub>2</sub> LiY, Cl <sub>6</sub> Cs <sub>2</sub> NaY, Cl <sub>6</sub> Cs <sub>2</sub> Pb, Cl <sub>6</sub> Cs <sub>2</sub> Pt, Cl <sub>6</sub> Cs <sub>2</sub> Se, Cl <sub>6</sub> Cs <sub>2</sub> Sn, Cl <sub>6</sub> Cs <sub>2</sub> Te, Cl <sub>6</sub> Cs <sub>2</sub> Ti, Cl <sub>6</sub> Cs <sub>2</sub> Zr, Cl <sub>6</sub> K <sub>2</sub> Pd, Cl <sub>6</sub> K <sub>2</sub> Pt, Cl <sub>6</sub> K <sub>2</sub> Sn, Cl <sub>6</sub> K <sub>2</sub> Ti, Cl <sub>6</sub> PbRb <sub>2</sub> , Cl <sub>6</sub> PtRb <sub>2</sub> , Cl <sub>6</sub> PtTl <sub>2</sub> , Cl <sub>6</sub> Rb <sub>2</sub> Se, Cl <sub>6</sub> Rb <sub>2</sub> Sn, Cl <sub>6</sub> Rb <sub>2</sub> Te, Cl <sub>6</sub> Rb <sub>2</sub> Ti, Cl <sub>6</sub> Rb <sub>2</sub> Zr, Cl <sub>6</sub> SnTl <sub>2</sub> , Cl <sub>6</sub> TeTl <sub>2</sub> , CsF <sub>3</sub> Tl, CsI, CsK <sub>2</sub> Sb, Cs <sub>2</sub> F <sub>6</sub> Ge, Cs <sub>2</sub> F <sub>6</sub> InNa, Cs <sub>2</sub> F <sub>6</sub> KY, Cs <sub>2</sub> F <sub>6</sub> NaSc, Cs <sub>2</sub> F <sub>6</sub> NaTl, Cs <sub>2</sub> F <sub>6</sub> NaY, Cs <sub>2</sub> F <sub>6</sub> Pd, Cs <sub>2</sub> F <sub>6</sub> Pt, Cs <sub>2</sub> F <sub>6</sub> RbY, Cs <sub>2</sub> F <sub>6</sub> Si, Cs <sub>2</sub> HfI <sub>6</sub> , Cs <sub>2</sub> I <sub>6</sub> Pd, Cs <sub>2</sub> I <sub>6</sub> Po, Cs <sub>2</sub> I <sub>6</sub> Pt, Cs <sub>2</sub> I <sub>6</sub> Sn, Cs <sub>2</sub> I <sub>6</sub> Te, Cs <sub>3</sub> Sb, Cs <sub>6</sub> I <sub>8</sub> Re <sub>6</sub> S <sub>8</sub> , F <sub>10</sub> KY <sub>3</sub> , F <sub>2</sub> Hg, F <sub>2</sub> Pb, F <sub>2</sub> Ra, F <sub>2</sub> Te, F <sub>3</sub> La, F <sub>6</sub> GaKRb <sub>2</sub> , F <sub>6</sub> GeRb <sub>2</sub> , F <sub>6</sub> HfK <sub>2</sub> , F <sub>6</sub> InKRb <sub>2</sub> , F <sub>6</sub> InK <sub>2</sub> Na, F <sub>6</sub> K <sub>2</sub> NaSc, F <sub>6</sub> K <sub>2</sub> NaTl, F <sub>6</sub> K <sub>2</sub> NaY, F <sub>6</sub> K <sub>2</sub> Si, F <sub>6</sub> NaRb <sub>2</sub> Y, F <sub>6</sub> NaSb, F <sub>6</sub> O <sub>4</sub> PbZr <sub>3</sub> , F <sub>6</sub> PdRb <sub>2</sub> , F <sub>6</sub> Rb <sub>2</sub> Si, F <sub>6</sub> SiTl <sub>2</sub> , F <sub>6</sub> Sn <sub>2</sub> , GaLiMg <sub>2</sub> , GaN, GaO <sub>6</sub> SbSr <sub>2</sub> , Ga <sub>2</sub> In <sub>6</sub> O <sub>8</sub> Pt, Ga <sub>4</sub> In <sub>3</sub> Sr <sub>11</sub> , Ge, GeMg <sub>2</sub> , GeTe, GeTh, Ge <sub>2</sub> In <sub>6</sub> O <sub>9</sub> Pt, He, HfO <sub>2</sub> , HgP <sub>2</sub> Si, HgS, IK, ILi, IRb, ITl, I <sub>6</sub> PdRb <sub>2</sub> , I <sub>6</sub> Rb <sub>2</sub> Sn, InN, InO <sub>6</sub> Sr <sub>2</sub> Ta, In <sub>7</sub> Sr <sub>11</sub> , KNa <sub>2</sub> Sb, LaP, LaSb, LiMg <sub>2</sub> Tl, Li <sub>2</sub> MgSi, Li <sub>2</sub> NaSb, Li <sub>2</sub> O, Li <sub>2</sub> S, Li <sub>2</sub> Se, Li <sub>2</sub> Te, Li <sub>3</sub> Sb, Li <sub>4</sub> N <sub>2</sub> Na <sub>2</sub> , LuN, LuSb, MgO, MgO <sub>6</sub> Pb <sub>2</sub> Te, MgO <sub>6</sub> Pb <sub>2</sub> W, MgO <sub>6</sub> Sr <sub>2</sub> W, MgS, MgSe, MgTe, Mg <sub>2</sub> Si, Mg <sub>2</sub> Sn, MoO <sub>6</sub> Sr <sub>2</sub> Zn, NPa, NSc, N <sub>2</sub> Pd, Na <sub>2</sub> S, Na <sub>2</sub> Se, Na <sub>2</sub> Te, Na <sub>6</sub> O <sub>9</sub> S <sub>2</sub> , OSr, OZn, O <sub>2</sub> Si, O <sub>2</sub> Sn, O <sub>2</sub> Ti, O <sub>2</sub> U, O <sub>2</sub> Zr, O <sub>4</sub> Pd <sub>3</sub> Tl, O <sub>6</sub> SbSr <sub>2</sub> Y, O <sub>6</sub> Sr <sub>2</sub> TaY, O <sub>6</sub> Sr <sub>2</sub> WZn, PSc, Pb, PbPo, PbS, PbSe, PbTe, PoSr, RaS, RaSe, Rb <sub>2</sub> S, Rb <sub>2</sub> Se, Rb <sub>2</sub> Te, Rn, S <sub>8</sub> Sn, SSr,

Part 25 of all the predicted materials with band crossings from **Cases 1 or 2**:

225	<chem>SbSc</chem> , <chem>SbY</chem> , <chem>SeSn</chem> , <chem>SeSr</chem> , <chem>SeU</chem> , <chem>SnTe</chem> , <chem>SrTe</chem> , <chem>TeU</chem> , <chem>TeZn</chem> , <chem>W</chem> , <chem>Xe</chem> , <chem>Y6Zn23</chem> ,
227	<chem>AgO3Sb</chem> , <chem>Ag2MoO4</chem> , <chem>Ag2O6Sb2</chem> , <chem>Ag3NaS2</chem> , <chem>Ag6K2S4</chem> , <chem>Al18Mg3Mo2</chem> , <chem>Al18Mg3W2</chem> , <chem>AlCsO2</chem> , <chem>AllLi</chem> , <chem>AlO2Rb</chem> , <chem>Al2Ba</chem> , <chem>Al2Ca</chem> , <chem>Al2CdO4</chem> , <chem>Al2CdSe4</chem> , <chem>Al2ClF25Sr10</chem> , <chem>Al2O4Zn</chem> , <chem>Al2Se4Zn</chem> , <chem>Al2Sr</chem> , <chem>Al2Th</chem> , <chem>As2O3</chem> , <chem>As4He2O6</chem> , <chem>As4NasTi</chem> , <chem>As4O6</chem> , <chem>BLi</chem> , <chem>Ba21O5Si2</chem> , <chem>Ba2Ge4S10</chem> , <chem>Be2Ti</chem> , <chem>Bi2O3</chem> , <chem>Bi2O7Pt2</chem> , <chem>Bi2O7Sn2</chem> , <chem>Bi2O7Ti2</chem> , <chem>CBr3LiN2Sr2</chem> , <chem>CNb4Zn2</chem> , <chem>CTi</chem> , <chem>CTi2</chem> , <chem>C3N4</chem> , <chem>C3Nb8Zn4</chem> , <chem>C4F12Ge4S6</chem> , <chem>Ca2Nb2O7</chem> , <chem>Ca2O7Sb2</chem> , <chem>Ca2O7Ta2</chem> , <chem>CdGa2O4</chem> , <chem>CdIn2O4</chem> , <chem>CdIn2S4</chem> , <chem>CdIn2Se4</chem> , <chem>CdLu2S4</chem> , <chem>CdLu2Se4</chem> , <chem>CdS4Sc2</chem> , <chem>CdS4Y2</chem> , <chem>CdSc2Se4</chem> , <chem>CdSe4Y2</chem> , <chem>Cd2Nb2O7</chem> , <chem>Cd2O4Si</chem> , <chem>Cd2O4Sn</chem> , <chem>Cd2O7Re2</chem> , <chem>Cd2O7Ta2</chem> , <chem>Cl4Li2Zn</chem> , <chem>CsN2Nb</chem> , <chem>F6Hg2OZn2</chem> , <chem>GaLi</chem> , <chem>Ga2MgO4</chem> , <chem>Ga2O4Zn</chem> , <chem>Ge136</chem> , <chem>GeMg2</chem> , <chem>GeMg2O4</chem> , <chem>Ge3N4</chem> , <chem>HfZn2</chem> , <chem>Hf2La2O7</chem> , <chem>Hf2O7Y2</chem> , <chem>Hf2Pd</chem> , <chem>Hf3NZn3</chem> , <chem>HgIn2S4</chem> , <chem>Hg2Nb2O7</chem> , <chem>Hg2O7Sb2</chem> , <chem>In2Mg</chem> , <chem>In2MgO4</chem> , <chem>In2O7Si2</chem> , <chem>In2S4Zn</chem> , <chem>In3Li13</chem> , <chem>KO3Sb</chem> , <chem>K8Sb4Sn</chem> , <chem>La2O7Sn2</chem> , <chem>La2O7Zr2</chem> , <chem>Lu2MgS4</chem> , <chem>Lu2MgSe4</chem> , <chem>Lu2O7Sn2</chem> , <chem>Lu2O7Ti2</chem> , <chem>MgS4Sc2</chem> , <chem>MgSc2Se4</chem> , <chem>MgSe4Y2</chem> , <chem>Mg2O4Si</chem> , <chem>Mg2O4Sn</chem> , <chem>Mg2Si</chem> , <chem>Mg2Sn</chem> , <chem>Mg2Th</chem> , <chem>MoNa2O4</chem> , <chem>Mo2O7Y2</chem> , <chem>NPd2Zr4</chem> , <chem>N4Si3</chem> , <chem>N4Sn3</chem> , <chem>NaTl</chem> , <chem>Na2O4W</chem> , <chem>Nb2O7Sn2</chem> , <chem>O3Sb2</chem> , <chem>O4SiZn2</chem> , <chem>O4SnZn2</chem> , <chem>O6Sb4</chem> , <chem>O7Sc2Si2</chem> , <chem>O7Sn2Ta2</chem> , <chem>O7Sn2Y2</chem> , <chem>O7Ti2Y2</chem> , <chem>Pd13Te3</chem> , <chem>S2Sn</chem> , <chem>S2Ti</chem> , <chem>S4Sc2Zn</chem> , <chem>S4Y2Zn</chem> , <chem>Se</chem> , <chem>Si136</chem> , <chem>Zn2Zr</chem> ,
229	<chem>B3Ba4N6Na</chem> , <chem>Ba2K8O24U6</chem> , <chem>Ba4NaO12Sb3</chem> , <chem>Be</chem> , <chem>CaK4O12U3</chem> , <chem>Ca2K8O24U6</chem> , <chem>F6Mo</chem> , <chem>F6S</chem> , <chem>Ge</chem> , <chem>He</chem> , <chem>Hg4Pt</chem> , <chem>K8O24Sr2U6</chem> ,
230	<chem>Al2Cd3O12Si3</chem> , <chem>Al2F12Li3Na3</chem> , <chem>Al5O12Y3</chem> , <chem>Al5O12Y3</chem> , <chem>B3Ba4NaO9</chem> , <chem>Bi6BrKO9</chem> , <chem>Ca3Ga2Ge3O12</chem> , <chem>Ca3Ga2O12Si3</chem> , <chem>Ca3Ge3O12Sc2</chem> , <chem>Cd3Ge3O12Sc2</chem> , <chem>Ga3Na3O12Te2</chem> , <chem>Ga5O12Y3</chem> , <chem>Ge3O12Sr3Y2</chem> , <chem>Hg3O6Te</chem> , <chem>O2Si</chem> , <chem>O2Si</chem> ,

## V. AI BASIS VECTORS FOR 230 SPACE GROUPS

$$\begin{pmatrix} \text{SG1} & a_1 \\ \nu & 2 \\ n_{\Gamma,1} & 1 \\ n_{X,1} & 1 \\ n_{Y,1} & 1 \\ n_{Z,1} & 1 \\ n_{U,1} & 1 \\ n_{T,1} & 1 \\ n_{S,1} & 1 \\ n_{R,1} & 1 \end{pmatrix} \quad (2)$$

$$\left( \begin{array}{ccccccccc} \text{SG2} & a_1 & a_2 & a_3 & a_4 & a_5 & a_6 & a_7 & a_8 & a_9 \\ \nu & 4 & 2 & 2 & 2 & 2 & -4 & -4 & -4 & 8 \\ n_{\Gamma,1} & 1 & 1 & 1 & 1 & 1 & -2 & -2 & -2 & 4 \\ n_{\Gamma,2} & 1 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ n_{X,1} & 1 & 1 & 0 & 1 & 0 & -2 & -2 & 0 & 4 \\ n_{X,2} & 1 & 0 & 1 & 0 & 1 & 0 & 0 & -2 & 0 \\ n_{Y,1} & 1 & 1 & 0 & 0 & 1 & -2 & 0 & -2 & 4 \\ n_{Y,2} & 1 & 0 & 1 & 1 & 0 & 0 & -2 & 0 & 0 \\ n_{Z,1} & 1 & 1 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ n_{Z,2} & 1 & 0 & 1 & 1 & 1 & -2 & -2 & -2 & 4 \\ n_{U,1} & 1 & 1 & 1 & 0 & 0 & 0 & -2 & -2 & 4 \\ n_{U,2} & 1 & 0 & 0 & 1 & 1 & -2 & 0 & 0 & 0 \\ n_{T,1} & 1 & 1 & 1 & 1 & 0 & -2 & -2 & -2 & 4 \\ n_{T,2} & 1 & 0 & 0 & 0 & 1 & 0 & 0 & 0 & 0 \\ n_{S,1} & 1 & 1 & 1 & 0 & 1 & -2 & -2 & -2 & 4 \\ n_{S,2} & 1 & 0 & 0 & 1 & 0 & 0 & 0 & 0 & 0 \\ n_{R,1} & 1 & 1 & 0 & 1 & 1 & -2 & -2 & -2 & 4 \\ n_{R,2} & 1 & 0 & 1 & 0 & 0 & 0 & 0 & 0 & 0 \end{array} \right) \quad (3)$$

$$\left( \begin{array}{cc} \text{SG3} & a_1 \\ \nu & 2 \\ n_{\Gamma,1} & 1 \\ n_{\Gamma,2} & 1 \\ n_{B,1} & 1 \\ n_{B,2} & 1 \\ n_{Y,1} & 1 \\ n_{Y,2} & 1 \\ n_{Z,1} & 1 \\ n_{Z,2} & 1 \\ n_{C,1} & 1 \\ n_{C,2} & 1 \\ n_{D,1} & 1 \\ n_{D,2} & 1 \\ n_{A,1} & 1 \\ n_{A,2} & 1 \\ n_{E,1} & 1 \\ n_{E,2} & 1 \end{array} \right) \quad (4)$$

$$\begin{pmatrix} \text{SG4} & a_1 \\ \nu & 4 \\ n_{\Gamma,1} & 2 \\ n_{\Gamma,2} & 2 \\ n_{B,1} & 2 \\ n_{B,2} & 2 \\ n_{Y,1} & 2 \\ n_{Y,2} & 2 \\ n_{Z,1} & 1 \\ n_{Z,2} & 1 \\ n_{C,1} & 1 \\ n_{C,2} & 1 \\ n_{D,1} & 1 \\ n_{D,2} & 1 \\ n_{A,1} & 2 \\ n_{A,2} & 2 \\ n_{E,1} & 1 \\ n_{E,2} & 1 \end{pmatrix} \quad (5)$$

$$\begin{pmatrix} \text{SG5} & a_1 \\ \nu & 2 \\ n_{\Gamma,1} & 1 \\ n_{\Gamma,2} & 1 \\ n_{A,1} & 1 \\ n_{A,2} & 1 \\ n_{Z,1} & 1 \\ n_{Z,2} & 1 \\ n_{M,1} & 1 \\ n_{M,2} & 1 \\ n_{L,1} & 1 \\ n_{V,1} & 1 \end{pmatrix} \quad (6)$$

$$\begin{pmatrix} \text{SG6} & a_1 \\ \nu & 2 \\ n_{\Gamma,1} & 1 \\ n_{\Gamma,2} & 1 \\ n_{B,1} & 1 \\ n_{B,2} & 1 \\ n_{Y,1} & 1 \\ n_{Y,2} & 1 \\ n_{Z,1} & 1 \\ n_{Z,2} & 1 \\ n_{C,1} & 1 \\ n_{C,2} & 1 \\ n_{D,1} & 1 \\ n_{D,2} & 1 \\ n_{A,1} & 1 \\ n_{A,2} & 1 \\ n_{E,1} & 1 \\ n_{E,2} & 1 \end{pmatrix} \quad (7)$$

$$\begin{pmatrix} \text{SG7} & a_1 \\ \nu & 4 \\ n_{\Gamma,1} & 2 \\ n_{\Gamma,2} & 2 \\ n_{B,1} & 1 \\ n_{B,2} & 1 \\ n_{Y,1} & 2 \\ n_{Y,2} & 2 \\ n_{Z,1} & 2 \\ n_{Z,2} & 2 \\ n_{C,1} & 2 \\ n_{C,2} & 2 \\ n_{D,1} & 1 \\ n_{D,2} & 1 \\ n_{A,1} & 1 \\ n_{A,2} & 1 \\ n_{E,1} & 1 \\ n_{E,2} & 1 \end{pmatrix} \quad (8)$$

$$\begin{pmatrix} \text{SG8} & a_1 \\ \nu & 2 \\ n_{\Gamma,1} & 1 \\ n_{\Gamma,2} & 1 \\ n_{A,1} & 1 \\ n_{A,2} & 1 \\ n_{Z,1} & 1 \\ n_{Z,2} & 1 \\ n_{M,1} & 1 \\ n_{M,2} & 1 \\ n_{L,1} & 1 \\ n_{V,1} & 1 \end{pmatrix} \quad (9)$$

$$\begin{pmatrix} \text{SG9} & a_1 \\ \nu & 4 \\ n_{\Gamma,1} & 2 \\ n_{\Gamma,2} & 2 \\ n_{A,1} & 1 \\ n_{A,2} & 1 \\ n_{Z,1} & 2 \\ n_{Z,2} & 2 \\ n_{M,1} & 1 \\ n_{M,2} & 1 \\ n_{L,1} & 2 \\ n_{V,1} & 2 \end{pmatrix} \quad (10)$$



$$\left( \begin{array}{cccccc} \text{SG11} & a_1 & a_2 & a_3 & a_4 & a_5 \\ \nu & 4 & 4 & 0 & 0 & 0 \\ n_{\Gamma,1} & 1 & 2 & 0 & 0 & 0 \\ n_{\Gamma,2} & 1 & 2 & 0 & 0 & 0 \\ n_{\Gamma,3} & 1 & 0 & 0 & 0 & 0 \\ n_{\Gamma,4} & 1 & 0 & 0 & 0 & 0 \\ n_{B,1} & 1 & 0 & 0 & 2 & 0 \\ n_{B,2} & 1 & 0 & 0 & 2 & 0 \\ n_{B,3} & 1 & 2 & 0 & -2 & 0 \\ n_{B,4} & 1 & 2 & 0 & -2 & 0 \\ n_{Y,1} & 1 & 0 & 2 & 0 & 0 \\ n_{Y,2} & 1 & 0 & 2 & 0 & 0 \\ n_{Y,3} & 1 & 2 & -2 & 0 & 0 \\ n_{Y,4} & 1 & 2 & -2 & 0 & 0 \\ n_{Z,1} & 1 & 1 & 0 & 0 & 0 \\ n_{C,1} & 1 & 1 & 0 & 0 & 0 \\ n_{D,1} & 1 & 1 & 0 & 0 & 0 \\ n_{A,1} & 1 & 2 & -2 & -2 & 4 \\ n_{A,2} & 1 & 2 & -2 & -2 & 4 \\ n_{A,3} & 1 & 0 & 2 & 2 & -4 \\ n_{A,4} & 1 & 0 & 2 & 2 & -4 \\ n_{E,1} & 1 & 1 & 0 & 0 & 0 \end{array} \right) \quad (12)$$

$$\left( \begin{array}{ccccccc} \text{SG12} & a_1 & a_2 & a_3 & a_4 & a_5 & a_6 & a_7 \\ \nu & 4 & 4 & -8 & 2 & -4 & 8 & -8 \\ n_{\Gamma,1} & 1 & 2 & -4 & 1 & -2 & 4 & -4 \\ n_{\Gamma,2} & 1 & 2 & -4 & 1 & -2 & 4 & -4 \\ n_{\Gamma,3} & 1 & 0 & 0 & 0 & 0 & 0 & 0 \\ n_{\Gamma,4} & 1 & 0 & 0 & 0 & 0 & 0 & 0 \\ n_{A,1} & 1 & 0 & -1 & 0 & 0 & 2 & -4 \\ n_{A,2} & 1 & 0 & -1 & 0 & 0 & 2 & -4 \\ n_{A,3} & 1 & 2 & -3 & 1 & -2 & 2 & 0 \\ n_{A,4} & 1 & 2 & -3 & 1 & -2 & 2 & 0 \\ n_{Z,1} & 1 & 0 & -2 & 1 & 0 & 2 & -4 \\ n_{Z,2} & 1 & 0 & -2 & 1 & 0 & 2 & -4 \\ n_{Z,3} & 1 & 2 & -2 & 0 & -2 & 2 & 0 \\ n_{Z,4} & 1 & 2 & -2 & 0 & -2 & 2 & 0 \\ n_{M,1} & 1 & 2 & -3 & 0 & -2 & 4 & 0 \\ n_{M,2} & 1 & 2 & -3 & 0 & -2 & 4 & 0 \\ n_{M,3} & 1 & 0 & -1 & 1 & 0 & 0 & -4 \\ n_{M,4} & 1 & 0 & -1 & 1 & 0 & 0 & -4 \\ n_{L,1} & 1 & 1 & -1 & 1 & -2 & 0 & 0 \\ n_{L,2} & 1 & 1 & -3 & 0 & 0 & 4 & -4 \\ n_{V,1} & 1 & 1 & 0 & 0 & 0 & 0 & 0 \\ n_{V,2} & 1 & 1 & -4 & 1 & -2 & 4 & -4 \end{array} \right) \quad (13)$$

$$\left( \begin{array}{cccccc} \text{SG13} & a_1 & a_2 & a_3 & a_4 & a_5 \\ \nu & 4 & 4 & 0 & 0 & 0 \\ n_{\Gamma,1} & 1 & 2 & 0 & 0 & 0 \\ n_{\Gamma,2} & 1 & 2 & 0 & 0 & 0 \\ n_{\Gamma,3} & 1 & 0 & 0 & 0 & 0 \\ n_{\Gamma,4} & 1 & 0 & 0 & 0 & 0 \\ n_{B,1} & 1 & 1 & 0 & 0 & 0 \\ n_{Y,1} & 1 & 0 & 2 & 0 & 0 \\ n_{Y,2} & 1 & 0 & 2 & 0 & 0 \\ n_{Y,3} & 1 & 2 & -2 & 0 & 0 \\ n_{Y,4} & 1 & 2 & -2 & 0 & 0 \\ n_{Z,1} & 1 & 2 & -2 & -2 & 4 \\ n_{Z,2} & 1 & 2 & -2 & -2 & 4 \\ n_{Z,3} & 1 & 0 & 2 & 2 & -4 \\ n_{Z,4} & 1 & 0 & 2 & 2 & -4 \\ n_{C,1} & 1 & 0 & 0 & 2 & 0 \\ n_{C,2} & 1 & 0 & 0 & 2 & 0 \\ n_{C,3} & 1 & 2 & 0 & -2 & 0 \\ n_{C,4} & 1 & 2 & 0 & -2 & 0 \\ n_{D,1} & 1 & 1 & 0 & 0 & 0 \\ n_{A,1} & 1 & 1 & 0 & 0 & 0 \\ n_{E,1} & 1 & 1 & 0 & 0 & 0 \end{array} \right) \quad (14)$$

$$\left( \begin{array}{cccccc} \text{SG14} & a_1 & a_2 & a_3 & a_4 & a_5 \\ \nu & 8 & 4 & 4 & -8 & -16 \\ n_{\Gamma,1} & 2 & 2 & 2 & -2 & -8 \\ n_{\Gamma,2} & 2 & 2 & 2 & -2 & -8 \\ n_{\Gamma,3} & 2 & 0 & 0 & -2 & 0 \\ n_{\Gamma,4} & 2 & 0 & 0 & -2 & 0 \\ n_{B,1} & 2 & 1 & 1 & -2 & -4 \\ n_{Y,1} & 2 & 0 & 2 & -2 & -4 \\ n_{Y,2} & 2 & 0 & 2 & -2 & -4 \\ n_{Y,3} & 2 & 2 & 0 & -2 & -4 \\ n_{Y,4} & 2 & 2 & 0 & -2 & -4 \\ n_{Z,1} & 2 & 1 & 1 & -2 & -4 \\ n_{C,1} & 2 & 1 & 1 & -2 & -4 \\ n_{D,1} & 1 & 1 & 1 & -2 & -4 \\ n_{D,2} & 1 & 1 & 1 & -2 & -4 \\ n_{D,3} & 1 & 0 & 0 & 0 & 0 \\ n_{D,4} & 1 & 0 & 0 & 0 & 0 \\ n_{A,1} & 2 & 1 & 1 & -2 & -4 \\ n_{E,1} & 1 & 0 & 1 & 0 & -4 \\ n_{E,2} & 1 & 0 & 1 & 0 & -4 \\ n_{E,3} & 1 & 1 & 0 & -2 & 0 \\ n_{E,4} & 1 & 1 & 0 & -2 & 0 \end{array} \right) \quad (15)$$

$$\left( \begin{array}{cccccc} \text{SG15} & a_1 & a_2 & a_3 & a_4 & a_5 \\ \nu & 4 & 4 & -12 & 16 & -16 \\ n_{\Gamma,1} & 1 & 2 & -6 & 8 & -8 \\ n_{\Gamma,2} & 1 & 2 & -6 & 8 & -8 \\ n_{\Gamma,3} & 1 & 0 & 0 & 0 & 0 \\ n_{\Gamma,4} & 1 & 0 & 0 & 0 & 0 \\ n_{A,1} & 1 & 1 & -3 & 4 & -4 \\ n_{Z,1} & 1 & 0 & -2 & 4 & -4 \\ n_{Z,2} & 1 & 0 & -2 & 4 & -4 \\ n_{Z,3} & 1 & 2 & -4 & 4 & -4 \\ n_{Z,4} & 1 & 2 & -4 & 4 & -4 \\ n_{M,1} & 1 & 1 & -3 & 4 & -4 \\ n_{L,1} & 1 & 2 & -5 & 6 & -4 \\ n_{L,2} & 1 & 0 & -1 & 2 & -4 \\ n_{V,1} & 1 & 1 & 0 & 0 & 0 \\ n_{V,2} & 1 & 1 & -6 & 8 & -8 \end{array} \right) \quad (16)$$

$$\left( \begin{array}{cc} \text{SG16} & a_1 \\ \nu & 2 \\ n_{\Gamma,1} & 1 \\ n_{Y,1} & 1 \\ n_{X,1} & 1 \\ n_{Z,1} & 1 \\ n_{U,1} & 1 \\ n_{T,1} & 1 \\ n_{S,1} & 1 \\ n_{R,1} & 1 \end{array} \right) \quad (17)$$

$$\left( \begin{array}{cc} \text{SG17} & a_1 \\ \nu & 4 \\ n_{\Gamma,1} & 2 \\ n_{Y,1} & 2 \\ n_{X,1} & 2 \\ n_{Z,1} & 1 \\ n_{Z,2} & 1 \\ n_{Z,3} & 1 \\ n_{Z,4} & 1 \\ n_{U,1} & 1 \\ n_{U,2} & 1 \\ n_{U,3} & 1 \\ n_{U,4} & 1 \\ n_{T,1} & 1 \\ n_{T,2} & 1 \\ n_{T,3} & 1 \\ n_{T,4} & 1 \\ n_{S,1} & 2 \\ n_{R,1} & 1 \\ n_{R,2} & 1 \\ n_{R,3} & 1 \\ n_{R,4} & 1 \end{array} \right) \quad (18)$$

$$\left( \begin{array}{ll} \text{SG18} & a_1 \\ \nu & 4 \\ n_{\Gamma,1} & 2 \\ n_{Y,1} & 1 \\ n_{Y,2} & 1 \\ n_{Y,3} & 1 \\ n_{Y,4} & 1 \\ n_{X,1} & 1 \\ n_{X,2} & 1 \\ n_{X,3} & 1 \\ n_{X,4} & 1 \\ n_{Z,1} & 2 \\ n_{U,1} & 1 \\ n_{U,2} & 1 \\ n_{U,3} & 1 \\ n_{U,4} & 1 \\ n_{T,1} & 1 \\ n_{T,2} & 1 \\ n_{T,3} & 1 \\ n_{T,4} & 1 \\ n_{S,1} & 1 \\ n_{R,1} & 1 \end{array} \right) \quad (19)$$

$$\left( \begin{array}{ll} \text{SG19} & a_1 \\ \nu & 8 \\ n_{\Gamma,1} & 4 \\ n_{Y,1} & 2 \\ n_{Y,2} & 2 \\ n_{Y,3} & 2 \\ n_{Y,4} & 2 \\ n_{X,1} & 2 \\ n_{X,2} & 2 \\ n_{X,3} & 2 \\ n_{X,4} & 2 \\ n_{Z,1} & 2 \\ n_{Z,2} & 2 \\ n_{Z,3} & 2 \\ n_{Z,4} & 2 \\ n_{U,1} & 2 \\ n_{T,1} & 2 \\ n_{S,1} & 2 \\ n_{R,1} & 1 \\ n_{R,2} & 1 \\ n_{R,3} & 1 \\ n_{R,4} & 1 \end{array} \right) \quad (20)$$

$$\begin{pmatrix} \text{SG20} & a_1 \\ \nu & 4 \\ n_{\Gamma,1} & 2 \\ n_{Y,1} & 2 \\ n_{Z,1} & 1 \\ n_{Z,2} & 1 \\ n_{Z,3} & 1 \\ n_{Z,4} & 1 \\ n_{T,1} & 1 \\ n_{T,2} & 1 \\ n_{T,3} & 1 \\ n_{T,4} & 1 \\ n_{S,1} & 2 \\ n_{S,2} & 2 \\ n_{R,1} & 1 \\ n_{R,2} & 1 \end{pmatrix} \quad (21)$$

$$\begin{pmatrix} \text{SG21} & a_1 \\ \nu & 2 \\ n_{\Gamma,1} & 1 \\ n_{Y,1} & 1 \\ n_{Z,1} & 1 \\ n_{T,1} & 1 \\ n_{S,1} & 1 \\ n_{S,2} & 0 \\ n_{R,1} & 1 \\ n_{R,2} & 0 \end{pmatrix} \quad (22)$$

$$\begin{pmatrix} \text{SG22} & a_1 \\ \nu & 2 \\ n_{\Gamma,1} & 1 \\ n_{Y,1} & 1 \\ n_{X,1} & 1 \\ n_{Z,1} & 1 \\ n_{L,1} & 1 \end{pmatrix} \quad (23)$$

$$\begin{pmatrix} \text{SG23} & a_1 \\ \nu & 2 \\ n_{\Gamma,1} & 1 \\ n_{X,1} & 1 \\ n_{R,1} & 1 \\ n_{R,2} & 1 \\ n_{S,1} & 1 \\ n_{S,2} & 1 \\ n_{T,1} & 1 \\ n_{T,2} & 1 \\ n_{W,1} & 1 \end{pmatrix} \quad (24)$$

$$\begin{pmatrix} \text{SG24} & a_1 \\ \nu & 4 \\ n_{\Gamma,1} & 2 \\ n_{X,1} & 2 \\ n_{R,1} & 2 \\ n_{R,2} & 2 \\ n_{S,1} & 2 \\ n_{S,2} & 2 \\ n_{T,1} & 2 \\ n_{T,2} & 2 \\ n_{W,1} & 1 \\ n_{W,2} & 1 \\ n_{W,3} & 1 \\ n_{W,4} & 1 \end{pmatrix} \quad (25)$$

$$\begin{pmatrix} \text{SG25} & a_1 \\ \nu & 2 \\ n_{\Gamma,1} & 1 \\ n_{Y,1} & 1 \\ n_{X,1} & 1 \\ n_{Z,1} & 1 \\ n_{U,1} & 1 \\ n_{T,1} & 1 \\ n_{S,1} & 1 \\ n_{R,1} & 1 \end{pmatrix} \quad (26)$$

$$\begin{pmatrix} \text{SG26} & a_1 \\ \nu & 2 \\ n_{\Gamma,1} & 1 \\ n_{Y,1} & 1 \\ n_{X,1} & 1 \\ n_{Z,1} & 1 \\ n_{U,1} & 1 \\ n_{T,1} & 1 \\ n_{S,1} & 1 \\ n_{R,1} & 1 \end{pmatrix} \quad (27)$$

$$\begin{pmatrix} \text{SG27} & a_1 \\ \nu & 2 \\ n_{\Gamma,1} & 1 \\ n_{Y,1} & 1 \\ n_{X,1} & 1 \\ n_{Z,1} & 1 \\ n_{U,1} & 1 \\ n_{T,1} & 1 \\ n_{S,1} & 1 \\ n_{R,1} & 1 \end{pmatrix} \quad (28)$$

$$\left( \begin{array}{ll} \text{SG28} & a_1 \\ \nu & 4 \\ n_{\Gamma,1} & 2 \\ n_{Y,1} & 1 \\ n_{Y,2} & 1 \\ n_{Y,3} & 1 \\ n_{Y,4} & 1 \\ n_{X,1} & 2 \\ n_{Z,1} & 2 \\ n_{U,1} & 2 \\ n_{T,1} & 1 \\ n_{T,2} & 1 \\ n_{T,3} & 1 \\ n_{T,4} & 1 \\ n_{S,1} & 1 \\ n_{S,2} & 1 \\ n_{S,3} & 1 \\ n_{S,4} & 1 \\ n_{R,1} & 1 \\ n_{R,2} & 1 \\ n_{R,3} & 1 \\ n_{R,4} & 1 \end{array} \right) \quad (29)$$

$$\left( \begin{array}{ll} \text{SG29} & a_1 \\ \nu & 8 \\ n_{\Gamma,1} & 4 \\ n_{Y,1} & 2 \\ n_{Y,2} & 2 \\ n_{Y,3} & 2 \\ n_{Y,4} & 2 \\ n_{X,1} & 4 \\ n_{Z,1} & 2 \\ n_{U,1} & 2 \\ n_{T,1} & 1 \\ n_{T,2} & 1 \\ n_{T,3} & 1 \\ n_{T,4} & 1 \\ n_{S,1} & 2 \\ n_{S,2} & 2 \\ n_{S,3} & 2 \\ n_{S,4} & 2 \\ n_{R,1} & 1 \\ n_{R,2} & 1 \\ n_{R,3} & 1 \\ n_{R,4} & 1 \end{array} \right) \quad (30)$$

$$\left( \begin{array}{cc} \text{SG30} & a_1 \\ \nu & 4 \\ n_{\Gamma,1} & 2 \\ n_{Y,1} & 1 \\ n_{Y,2} & 1 \\ n_{Y,3} & 1 \\ n_{Y,4} & 1 \\ n_{X,1} & 2 \\ n_{Z,1} & 1 \\ n_{U,1} & 1 \\ n_{T,1} & 1 \\ n_{T,2} & 1 \\ n_{T,3} & 1 \\ n_{T,4} & 1 \\ n_{S,1} & 1 \\ n_{S,2} & 1 \\ n_{S,3} & 1 \\ n_{S,4} & 1 \\ n_{R,1} & 1 \\ n_{R,2} & 1 \\ n_{R,3} & 1 \\ n_{R,4} & 1 \end{array} \right) \quad (31)$$

$$\left( \begin{array}{cc} \text{SG31} & a_1 \\ \nu & 4 \\ n_{\Gamma,1} & 2 \\ n_{Y,1} & 1 \\ n_{Y,2} & 1 \\ n_{Y,3} & 1 \\ n_{Y,4} & 1 \\ n_{X,1} & 2 \\ n_{Z,1} & 1 \\ n_{U,1} & 1 \\ n_{T,1} & 1 \\ n_{T,2} & 1 \\ n_{T,3} & 1 \\ n_{T,4} & 1 \\ n_{S,1} & 1 \\ n_{S,2} & 1 \\ n_{S,3} & 1 \\ n_{S,4} & 1 \\ n_{R,1} & 1 \\ n_{R,2} & 1 \\ n_{R,3} & 1 \\ n_{R,4} & 1 \end{array} \right) \quad (32)$$

$$\left( \begin{array}{cc} \text{SG32} & a_1 \\ \nu & 4 \\ n_{\Gamma,1} & 2 \\ n_{Y,1} & 1 \\ n_{Y,2} & 1 \\ n_{Y,3} & 1 \\ n_{Y,4} & 1 \\ n_{X,1} & 1 \\ n_{X,2} & 1 \\ n_{X,3} & 1 \\ n_{X,4} & 1 \\ n_{Z,1} & 2 \\ n_{U,1} & 1 \\ n_{U,2} & 1 \\ n_{U,3} & 1 \\ n_{U,4} & 1 \\ n_{T,1} & 1 \\ n_{T,2} & 1 \\ n_{T,3} & 1 \\ n_{T,4} & 1 \\ n_{S,1} & 1 \\ n_{R,1} & 1 \end{array} \right) \quad (33)$$

$$\left( \begin{array}{cc} \text{SG33} & a_1 \\ \nu & 8 \\ n_{\Gamma,1} & 4 \\ n_{Y,1} & 2 \\ n_{Y,2} & 2 \\ n_{Y,3} & 2 \\ n_{Y,4} & 2 \\ n_{X,1} & 2 \\ n_{X,2} & 2 \\ n_{X,3} & 2 \\ n_{X,4} & 2 \\ n_{Z,1} & 2 \\ n_{U,1} & 2 \\ n_{U,2} & 2 \\ n_{U,3} & 2 \\ n_{U,4} & 2 \\ n_{T,1} & 1 \\ n_{T,2} & 1 \\ n_{T,3} & 1 \\ n_{T,4} & 1 \\ n_{S,1} & 2 \\ n_{R,1} & 2 \end{array} \right) \quad (34)$$

$$\begin{pmatrix} \text{SG34} & a_1 \\ \nu & 4 \\ n_{\Gamma,1} & 2 \\ n_{Y,1} & 1 \\ n_{Y,2} & 1 \\ n_{Y,3} & 1 \\ n_{Y,4} & 1 \\ n_{X,1} & 1 \\ n_{X,2} & 1 \\ n_{X,3} & 1 \\ n_{X,4} & 1 \\ n_{Z,1} & 1 \\ n_{U,1} & 1 \\ n_{U,2} & 1 \\ n_{U,3} & 1 \\ n_{U,4} & 1 \\ n_{T,1} & 1 \\ n_{T,2} & 1 \\ n_{T,3} & 1 \\ n_{T,4} & 1 \\ n_{S,1} & 1 \\ n_{R,1} & 2 \end{pmatrix} \quad (35)$$

$$\begin{pmatrix} \text{SG35} & a_1 \\ \nu & 2 \\ n_{\Gamma,1} & 1 \\ n_{Y,1} & 1 \\ n_{Z,1} & 1 \\ n_{T,1} & 1 \\ n_{S,1} & 1 \\ n_{S,2} & 1 \\ n_{R,1} & 1 \\ n_{R,2} & 1 \end{pmatrix} \quad (36)$$

$$\begin{pmatrix} \text{SG36} & a_1 \\ \nu & 4 \\ n_{\Gamma,1} & 2 \\ n_{Y,1} & 2 \\ n_{Z,1} & 1 \\ n_{T,1} & 1 \\ n_{S,1} & 2 \\ n_{S,2} & 2 \\ n_{R,1} & 1 \\ n_{R,2} & 1 \end{pmatrix} \quad (37)$$

$$\begin{pmatrix} \text{SG37} & a_1 \\ \nu & 4 \\ n_{\Gamma,1} & 2 \\ n_{Y,1} & 2 \\ n_{Z,1} & 1 \\ n_{T,1} & 1 \\ n_{S,1} & 2 \\ n_{S,2} & 2 \\ n_{R,1} & 2 \\ n_{R,2} & 2 \end{pmatrix} \quad (38)$$

$$\begin{pmatrix} \text{SG38} & a_1 \\ \nu & 2 \\ n_{\Gamma,1} & 1 \\ n_{Y,1} & 1 \\ n_{Z,1} & 1 \\ n_{T,1} & 1 \\ n_{S,1} & 1 \\ n_{S,2} & 1 \\ n_{R,1} & 1 \\ n_{R,2} & 1 \end{pmatrix} \quad (39)$$

$$\begin{pmatrix} \text{SG39} & a_1 \\ \nu & 4 \\ n_{\Gamma,1} & 2 \\ n_{Y,1} & 2 \\ n_{X,1} & 2 \\ n_{T,1} & 2 \\ n_{S,1} & 1 \\ n_{S,2} & 1 \\ n_{R,1} & 1 \\ n_{R,2} & 1 \end{pmatrix} \quad (40)$$

$$\begin{pmatrix} \text{SG40} & a_1 \\ \nu & 4 \\ n_{\Gamma,1} & 2 \\ n_{Y,1} & 2 \\ n_{Z,1} & 1 \\ n_{Z,2} & 1 \\ n_{Z,3} & 1 \\ n_{Z,4} & 1 \\ n_{T,1} & 1 \\ n_{T,2} & 1 \\ n_{T,3} & 1 \\ n_{T,4} & 1 \\ n_{S,1} & 2 \\ n_{S,2} & 2 \\ n_{R,1} & 2 \\ n_{R,2} & 2 \end{pmatrix} \quad (41)$$

$$\begin{pmatrix} \text{SG41} & a_1 \\ \nu & 4 \\ n_{\Gamma,1} & 2 \\ n_{Y,1} & 2 \\ n_{Z,1} & 1 \\ n_{Z,2} & 1 \\ n_{Z,3} & 1 \\ n_{Z,4} & 1 \\ n_{T,1} & 1 \\ n_{T,2} & 1 \\ n_{T,3} & 1 \\ n_{T,4} & 1 \\ n_{S,1} & 1 \\ n_{S,2} & 1 \\ n_{R,1} & 1 \\ n_{R,2} & 1 \end{pmatrix} \quad (42)$$

$$\begin{pmatrix} \text{SG42} & a_1 \\ \nu & 2 \\ n_{\Gamma,1} & 1 \\ n_{Y,1} & 1 \\ n_{X,1} & 1 \\ n_{Z,1} & 1 \\ n_{L,1} & 1 \end{pmatrix} \quad (43)$$

$$\begin{pmatrix} \text{SG43} & a_1 \\ \nu & 4 \\ n_{\Gamma,1} & 2 \\ n_{Y,1} & 1 \\ n_{Y,2} & 1 \\ n_{Y,3} & 1 \\ n_{Y,4} & 1 \\ n_{X,1} & 1 \\ n_{X,2} & 1 \\ n_{X,3} & 1 \\ n_{X,4} & 1 \\ n_{Z,1} & 1 \\ n_{L,1} & 2 \end{pmatrix} \quad (44)$$

$$\begin{pmatrix} \text{SG43} & a_1 \\ \nu & 2 \\ n_{\Gamma,1} & 1 \\ n_{X,1} & 1 \\ n_{R,1} & 1 \\ n_{R,2} & 1 \\ n_{S,1} & 1 \\ n_{S,2} & 1 \\ n_{T,1} & 1 \\ n_{T,2} & 1 \\ n_{W,1} & 1 \\ n_{W,2} & 1 \end{pmatrix} \quad (45)$$

$$\begin{pmatrix} \text{SG45} & a_1 \\ \nu & 4 \\ n_{\Gamma,1} & 2 \\ n_{X,1} & 2 \\ n_{R,1} & 1 \\ n_{R,2} & 1 \\ n_{S,1} & 1 \\ n_{S,2} & 1 \\ n_{T,1} & 2 \\ n_{T,2} & 2 \\ n_{W,1} & 1 \\ n_{W,2} & 1 \end{pmatrix} \quad (46)$$

$$\begin{pmatrix} \text{SG46} & a_1 \\ \nu & 4 \\ n_{\Gamma,1} & 2 \\ n_{X,1} & 2 \\ n_{R,1} & 2 \\ n_{R,2} & 2 \\ n_{S,1} & 1 \\ n_{S,2} & 1 \\ n_{T,1} & 2 \\ n_{T,2} & 2 \\ n_{W,1} & 2 \\ n_{W,2} & 2 \end{pmatrix} \quad (47)$$

$$\begin{pmatrix} \text{SG47} & a_1 & a_2 & a_3 & a_4 & a_5 & a_6 & a_7 & a_8 & a_9 \\ \nu & 4 & 2 & 2 & 2 & -2 & 4 & -4 & -4 & 8 \\ n_{\Gamma,1} & 1 & 1 & 1 & 1 & -1 & 2 & -2 & -2 & 4 \\ n_{\Gamma,2} & 1 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ n_{Y,1} & 1 & 0 & 1 & 0 & 0 & 0 & 0 & 0 & 0 \\ n_{Y,2} & 1 & 1 & 0 & 1 & -1 & 2 & -2 & -2 & 4 \\ n_{X,1} & 1 & 0 & 0 & 0 & 1 & 0 & 0 & 0 & 0 \\ n_{X,2} & 1 & 1 & 1 & 1 & -2 & 2 & -2 & -2 & 4 \\ n_{Z,1} & 1 & 0 & 0 & 1 & 0 & 0 & 0 & 0 & 0 \\ n_{Z,2} & 1 & 1 & 1 & 0 & -1 & 2 & -2 & -2 & 4 \\ n_{U,1} & 1 & 1 & 1 & 0 & 0 & 0 & -2 & 0 & 4 \\ n_{U,2} & 1 & 0 & 0 & 1 & -1 & 2 & 0 & -2 & 0 \\ n_{T,1} & 1 & 1 & 0 & 0 & 1 & 0 & -2 & -2 & 4 \\ n_{T,2} & 1 & 0 & 1 & 1 & -2 & 2 & 0 & 0 & 0 \\ n_{S,1} & 1 & 1 & 0 & 1 & 0 & 0 & 0 & -2 & 4 \\ n_{S,2} & 1 & 0 & 1 & 0 & -1 & 2 & -2 & 0 & 0 \\ n_{R,1} & 1 & 0 & 1 & 1 & -1 & 2 & -2 & -2 & 4 \\ n_{R,2} & 1 & 1 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \end{pmatrix} \quad (48)$$

$$\begin{pmatrix} \text{SG48} & a_1 & a_2 & a_3 \\ \nu & 4 & 8 & 0 \\ n_{\Gamma,1} & 1 & 4 & 0 \\ n_{\Gamma,2} & 1 & 0 & 0 \\ n_{Y,1} & 1 & 2 & 0 \\ n_{Y,2} & 1 & 2 & 0 \\ n_{X,1} & 1 & 2 & 0 \\ n_{X,2} & 1 & 2 & 0 \\ n_{Z,1} & 1 & 2 & 0 \\ n_{Z,2} & 1 & 2 & 0 \\ n_{U,1} & 1 & 2 & 0 \\ n_{U,2} & 1 & 2 & 0 \\ n_{T,1} & 1 & 2 & 0 \\ n_{T,2} & 1 & 2 & 0 \\ n_{S,1} & 1 & 2 & 0 \\ n_{S,2} & 1 & 2 & 0 \\ n_{R,1} & 1 & 4 & -4 \\ n_{R,2} & 1 & 0 & 4 \end{pmatrix} \quad (49)$$

$$\begin{pmatrix} \text{SG49} & a_1 & a_2 & a_3 & a_4 & a_5 \\ \nu & 4 & 4 & 0 & 0 & 0 \\ n_{\Gamma,1} & 1 & 2 & 0 & 0 & 0 \\ n_{\Gamma,2} & 1 & 0 & 0 & 0 & 0 \\ n_{Y,1} & 1 & 2 & -2 & -2 & 4 \\ n_{Y,2} & 1 & 0 & 2 & 2 & -4 \\ n_{X,1} & 1 & 0 & 2 & 0 & 0 \\ n_{X,2} & 1 & 2 & -2 & 0 & 0 \\ n_{Z,1} & 1 & 1 & 0 & 0 & 0 \\ n_{Z,2} & 1 & 1 & 0 & 0 & 0 \\ n_{U,1} & 1 & 1 & 0 & 0 & 0 \\ n_{U,2} & 1 & 1 & 0 & 0 & 0 \\ n_{T,1} & 1 & 1 & 0 & 0 & 0 \\ n_{T,2} & 1 & 1 & 0 & 0 & 0 \\ n_{S,1} & 1 & 0 & 0 & 2 & 0 \\ n_{S,2} & 1 & 2 & 0 & -2 & 0 \\ n_{R,1} & 1 & 1 & 0 & 0 & 0 \\ n_{R,2} & 1 & 1 & 0 & 0 & 0 \end{pmatrix} \quad (50)$$

$$\begin{pmatrix} \text{SG50} & a_1 & a_2 & a_3 \\ \nu & 4 & 8 & 0 \\ n_{\Gamma,1} & 1 & 4 & 0 \\ n_{\Gamma,2} & 1 & 0 & 0 \\ n_{Y,1} & 1 & 2 & 0 \\ n_{Y,2} & 1 & 2 & 0 \\ n_{X,1} & 1 & 2 & 0 \\ n_{X,2} & 1 & 2 & 0 \\ n_{Z,1} & 1 & 0 & 4 \\ n_{Z,2} & 1 & 4 & -4 \\ n_{U,1} & 1 & 2 & 0 \\ n_{U,2} & 1 & 2 & 0 \\ n_{T,1} & 1 & 2 & 0 \\ n_{T,2} & 1 & 2 & 0 \\ n_{S,1} & 1 & 2 & 0 \\ n_{S,2} & 1 & 2 & 0 \\ n_{R,1} & 1 & 2 & 0 \\ n_{R,2} & 1 & 2 & 0 \end{pmatrix} \quad (51)$$

$$\begin{pmatrix} \text{SG51} & a_1 & a_2 & a_3 & a_4 & a_5 \\ \nu & 4 & 4 & 0 & 0 & 0 \\ n_{\Gamma,1} & 1 & 2 & 0 & 0 & 0 \\ n_{\Gamma,2} & 1 & 0 & 0 & 0 & 0 \\ n_{Y,1} & 1 & 0 & 2 & 0 & 0 \\ n_{Y,2} & 1 & 2 & -2 & 0 & 0 \\ n_{X,1} & 1 & 0 & 0 & 2 & 0 \\ n_{X,2} & 1 & 2 & 0 & -2 & 0 \\ n_{Z,1} & 1 & 1 & 0 & 0 & 0 \\ n_{Z,2} & 1 & 1 & 0 & 0 & 0 \\ n_{U,1} & 1 & 1 & 0 & 0 & 0 \\ n_{U,2} & 1 & 1 & 0 & 0 & 0 \\ n_{T,1} & 1 & 1 & 0 & 0 & 0 \\ n_{T,2} & 1 & 1 & 0 & 0 & 0 \\ n_{S,1} & 1 & 2 & -2 & -2 & 4 \\ n_{S,2} & 1 & 0 & 2 & 2 & -4 \\ n_{R,1} & 1 & 1 & 0 & 0 & 0 \\ n_{R,2} & 1 & 1 & 0 & 0 & 0 \end{pmatrix} \quad (52)$$

$$\left( \begin{array}{ccccc} \text{SG52} & a_1 & a_2 & a_3 \\ \nu & 8 & 8 & -32 \\ n_{\Gamma,1} & 2 & 4 & -12 \\ n_{\Gamma,2} & 2 & 0 & -4 \\ n_{Y,1} & 2 & 2 & -8 \\ n_{Y,2} & 2 & 2 & -8 \\ n_{X,1} & 2 & 2 & -8 \\ n_{X,2} & 2 & 2 & -8 \\ n_{Z,1} & 2 & 2 & -8 \\ n_{Z,2} & 2 & 2 & -8 \\ n_{U,1} & 1 & 1 & -4 \\ n_{U,2} & 1 & 1 & -4 \\ n_{T,1} & 1 & 0 & 0 \\ n_{T,2} & 1 & 0 & 0 \\ n_{T,3} & 1 & 0 & 0 \\ n_{T,4} & 1 & 0 & 0 \\ n_{T,5} & 1 & 2 & -8 \\ n_{T,6} & 1 & 2 & -8 \\ n_{T,7} & 1 & 2 & -8 \\ n_{T,8} & 1 & 2 & -8 \\ n_{S,1} & 2 & 2 & -8 \\ n_{S,2} & 2 & 2 & -8 \\ n_{R,1} & 2 & 2 & -8 \\ n_{R,2} & 2 & 2 & -8 \end{array} \right) \quad (53)$$

$$\left( \begin{array}{cccccc} \text{SG53} & a_1 & a_2 & a_3 & a_4 & a_5 \\ \nu & 8 & 4 & -20 & 24 & -16 \\ n_{\Gamma,1} & 2 & 2 & -8 & 10 & -8 \\ n_{\Gamma,2} & 2 & 0 & -2 & 2 & 0 \\ n_{Y,1} & 2 & 1 & -5 & 6 & -4 \\ n_{Y,2} & 2 & 1 & -5 & 6 & -4 \\ n_{X,1} & 2 & 0 & -4 & 6 & -4 \\ n_{X,2} & 2 & 2 & -6 & 6 & -4 \\ n_{Z,1} & 2 & 1 & -5 & 6 & -4 \\ n_{Z,2} & 2 & 1 & -5 & 6 & -4 \\ n_{U,1} & 2 & 1 & -5 & 6 & -4 \\ n_{U,2} & 2 & 1 & -5 & 6 & -4 \\ n_{T,1} & 1 & 0 & -3 & 4 & -4 \\ n_{T,2} & 1 & 0 & -3 & 4 & -4 \\ n_{T,3} & 1 & 0 & -3 & 4 & -4 \\ n_{T,4} & 1 & 0 & -3 & 4 & -4 \\ n_{T,5} & 1 & 1 & -2 & 2 & 0 \\ n_{T,6} & 1 & 1 & -2 & 2 & 0 \\ n_{T,7} & 1 & 1 & -2 & 2 & 0 \\ n_{T,8} & 1 & 1 & -2 & 2 & 0 \\ n_{S,1} & 2 & 1 & -5 & 6 & -4 \\ n_{S,2} & 2 & 1 & -5 & 6 & -4 \\ n_{R,1} & 1 & 1 & -5 & 6 & -4 \\ n_{R,2} & 1 & 1 & -5 & 6 & -4 \\ n_{R,3} & 1 & 1 & -5 & 6 & -4 \\ n_{R,4} & 1 & 1 & -5 & 6 & -4 \\ n_{R,5} & 1 & 0 & 0 & 0 & 0 \\ n_{R,6} & 1 & 0 & 0 & 0 & 0 \\ n_{R,7} & 1 & 0 & 0 & 0 & 0 \\ n_{R,8} & 1 & 0 & 0 & 0 & 0 \end{array} \right) \quad (54)$$

$$\begin{pmatrix} \text{SG54} & a_1 & a_2 & a_3 \\ \nu & 8 & 0 & 0 \\ n_{\Gamma,1} & 2 & 2 & 0 \\ n_{\Gamma,2} & 2 & -2 & 0 \\ n_{Y,1} & 2 & -2 & 4 \\ n_{Y,2} & 2 & 2 & -4 \\ n_{X,1} & 2 & 0 & 0 \\ n_{X,2} & 2 & 0 & 0 \\ n_{Z,1} & 2 & 0 & 0 \\ n_{Z,2} & 2 & 0 & 0 \\ n_{U,1} & 1 & 0 & 0 \\ n_{U,2} & 1 & 0 & 0 \\ n_{T,1} & 2 & 0 & 0 \\ n_{T,2} & 2 & 0 & 0 \\ n_{S,1} & 2 & 0 & 0 \\ n_{S,2} & 2 & 0 & 0 \\ n_{R,1} & 1 & 0 & 0 \\ n_{R,2} & 1 & 0 & 0 \end{pmatrix} \quad (55)$$

$$\begin{pmatrix} \text{SG55} & a_1 & a_2 & a_3 & a_4 & a_5 \\ \nu & 8 & 4 & 4 & -8 & -16 \\ n_{\Gamma,1} & 2 & 2 & 2 & -2 & -8 \\ n_{\Gamma,2} & 2 & 0 & 0 & -2 & 0 \\ n_{Y,1} & 2 & 1 & 1 & -2 & -4 \\ n_{Y,2} & 2 & 1 & 1 & -2 & -4 \\ n_{X,1} & 2 & 1 & 1 & -2 & -4 \\ n_{X,2} & 2 & 1 & 1 & -2 & -4 \\ n_{Z,1} & 2 & 0 & 2 & -2 & -4 \\ n_{Z,2} & 2 & 2 & 0 & -2 & -4 \\ n_{U,1} & 2 & 1 & 1 & -2 & -4 \\ n_{U,2} & 2 & 1 & 1 & -2 & -4 \\ n_{T,1} & 2 & 1 & 1 & -2 & -4 \\ n_{T,2} & 2 & 1 & 1 & -2 & -4 \\ n_{S,1} & 1 & 0 & 0 & 0 & 0 \\ n_{S,2} & 1 & 1 & 1 & -2 & -4 \\ n_{R,1} & 1 & 1 & 0 & -2 & 0 \\ n_{R,2} & 1 & 0 & 1 & 0 & -4 \end{pmatrix} \quad (56)$$

$$\left( \begin{array}{cccc} \text{SG56} & a_1 & a_2 & a_3 \\ \nu & 8 & 8 & -32 \\ n_{\Gamma,1} & 2 & 4 & -12 \\ n_{\Gamma,2} & 2 & 0 & -4 \\ n_{Y,1} & 2 & 2 & -8 \\ n_{Y,2} & 2 & 2 & -8 \\ n_{X,1} & 2 & 2 & -8 \\ n_{X,2} & 2 & 2 & -8 \\ n_{Z,1} & 2 & 2 & -8 \\ n_{Z,2} & 2 & 2 & -8 \\ n_{U,1} & 1 & 1 & -4 \\ n_{U,2} & 1 & 1 & -4 \\ n_{T,1} & 1 & 1 & -4 \\ n_{T,2} & 1 & 1 & -4 \\ n_{S,1} & 2 & 2 & -8 \\ n_{S,2} & 2 & 2 & -8 \\ n_{R,1} & 1 & 2 & -8 \\ n_{R,2} & 1 & 0 & 0 \end{array} \right) \quad (57)$$

$$\left( \begin{array}{cccc} \text{SG57} & a_1 & a_2 & a_3 \\ \nu & 8 & 0 & 0 \\ n_{\Gamma,1} & 2 & 2 & 0 \\ n_{\Gamma,2} & 2 & -2 & 0 \\ n_{Y,1} & 2 & 0 & 0 \\ n_{Y,2} & 2 & 0 & 0 \\ n_{X,1} & 2 & 0 & 0 \\ n_{X,2} & 2 & 0 & 0 \\ n_{Z,1} & 2 & -2 & 4 \\ n_{Z,2} & 2 & 2 & -4 \\ n_{U,1} & 2 & 0 & 0 \\ n_{U,2} & 2 & 0 & 0 \\ n_{T,1} & 2 & 0 & 0 \\ n_{T,2} & 2 & 0 & 0 \\ n_{S,1} & 1 & 0 & 0 \\ n_{S,2} & 1 & 0 & 0 \\ n_{R,1} & 1 & 0 & 0 \\ n_{R,2} & 1 & 0 & 0 \end{array} \right) \quad (58)$$

$$\left( \begin{array}{l} \text{SG58} \quad a_1 \quad a_2 \quad a_3 \quad a_4 \quad a_5 \\ \nu \quad 8 \quad 4 \quad 4 \quad 4 \quad -48 \\ n_{\Gamma,1} \quad 2 \quad 2 \quad 2 \quad 2 \quad -20 \\ n_{\Gamma,2} \quad 2 \quad 0 \quad 0 \quad 0 \quad -4 \\ n_{Y,1} \quad 2 \quad 1 \quad 1 \quad 1 \quad -12 \\ n_{Y,2} \quad 2 \quad 1 \quad 1 \quad 1 \quad -12 \\ n_{X,1} \quad 2 \quad 1 \quad 1 \quad 1 \quad -12 \\ n_{X,2} \quad 2 \quad 1 \quad 1 \quad 1 \quad -12 \\ n_{Z,1} \quad 2 \quad 1 \quad 1 \quad 1 \quad -12 \\ n_{Z,2} \quad 2 \quad 1 \quad 1 \quad 1 \quad -12 \\ n_{U,1} \quad 1 \quad 1 \quad 0 \quad 1 \quad -8 \\ n_{U,2} \quad 1 \quad 1 \quad 0 \quad 1 \quad -8 \\ n_{U,3} \quad 1 \quad 1 \quad 0 \quad 1 \quad -8 \\ n_{U,4} \quad 1 \quad 1 \quad 0 \quad 1 \quad -8 \\ n_{U,5} \quad 1 \quad 0 \quad 1 \quad 0 \quad -4 \\ n_{U,6} \quad 1 \quad 0 \quad 1 \quad 0 \quad -4 \\ n_{U,7} \quad 1 \quad 0 \quad 1 \quad 0 \quad -4 \\ n_{U,8} \quad 1 \quad 0 \quad 1 \quad 0 \quad -4 \\ n_{T,1} \quad 1 \quad 0 \quad 1 \quad 1 \quad -8 \\ n_{T,2} \quad 1 \quad 0 \quad 1 \quad 1 \quad -8 \\ n_{T,3} \quad 1 \quad 0 \quad 1 \quad 1 \quad -8 \\ n_{T,4} \quad 1 \quad 0 \quad 1 \quad 1 \quad -8 \\ n_{T,5} \quad 1 \quad 1 \quad 0 \quad 0 \quad -4 \\ n_{T,6} \quad 1 \quad 1 \quad 0 \quad 0 \quad -4 \\ n_{T,7} \quad 1 \quad 1 \quad 0 \quad 0 \quad -4 \\ n_{T,8} \quad 1 \quad 1 \quad 0 \quad 0 \quad -4 \\ n_{S,1} \quad 1 \quad 0 \quad 0 \quad 1 \quad -4 \\ n_{S,2} \quad 1 \quad 1 \quad 1 \quad 0 \quad -8 \\ n_{R,1} \quad 2 \quad 1 \quad 1 \quad 1 \quad -12 \\ n_{R,2} \quad 2 \quad 1 \quad 1 \quad 1 \quad -12 \end{array} \right) \quad (59)$$

$$\left( \begin{array}{l} \text{SG59} \quad a_1 \quad a_2 \quad a_3 \\ \nu \quad 4 \quad 8 \quad 0 \\ n_{\Gamma,1} \quad 1 \quad 4 \quad 0 \\ n_{\Gamma,2} \quad 1 \quad 0 \quad 0 \\ n_{Y,1} \quad 1 \quad 2 \quad 0 \\ n_{Y,2} \quad 1 \quad 2 \quad 0 \\ n_{X,1} \quad 1 \quad 2 \quad 0 \\ n_{X,2} \quad 1 \quad 2 \quad 0 \\ n_{Z,1} \quad 1 \quad 0 \quad 4 \\ n_{Z,2} \quad 1 \quad 4 \quad -4 \\ n_{U,1} \quad 1 \quad 2 \quad 0 \\ n_{U,2} \quad 1 \quad 2 \quad 0 \\ n_{T,1} \quad 1 \quad 2 \quad 0 \\ n_{T,2} \quad 1 \quad 2 \quad 0 \\ n_{S,1} \quad 1 \quad 2 \quad 0 \\ n_{S,2} \quad 1 \quad 2 \quad 0 \\ n_{R,1} \quad 1 \quad 2 \quad 0 \\ n_{R,2} \quad 1 \quad 2 \quad 0 \end{array} \right) \quad (60)$$

$$\left( \begin{array}{l} \text{SG60} \quad a_1 \quad a_2 \quad a_3 \\ \nu \quad 8 \quad 8 \quad -32 \\ n_{\Gamma,1} \quad 2 \quad 4 \quad -12 \\ n_{\Gamma,2} \quad 2 \quad 0 \quad -4 \\ n_{Y,1} \quad 2 \quad 2 \quad -8 \\ n_{Y,2} \quad 2 \quad 2 \quad -8 \\ n_{X,1} \quad 2 \quad 2 \quad -8 \\ n_{X,2} \quad 2 \quad 2 \quad -8 \\ n_{Z,1} \quad 2 \quad 2 \quad -8 \\ n_{Z,2} \quad 2 \quad 2 \quad -8 \\ n_{U,1} \quad 1 \quad 0 \quad 0 \\ n_{U,2} \quad 1 \quad 0 \quad 0 \\ n_{U,3} \quad 1 \quad 0 \quad 0 \\ n_{U,4} \quad 1 \quad 0 \quad 0 \\ n_{U,5} \quad 1 \quad 2 \quad -8 \\ n_{U,6} \quad 1 \quad 2 \quad -8 \\ n_{U,7} \quad 1 \quad 2 \quad -8 \\ n_{U,8} \quad 1 \quad 2 \quad -8 \\ n_{T,1} \quad 1 \quad 1 \quad -4 \\ n_{T,2} \quad 1 \quad 1 \quad -4 \\ n_{S,1} \quad 1 \quad 1 \quad -4 \\ n_{S,2} \quad 1 \quad 1 \quad -4 \\ n_{R,1} \quad 1 \quad 1 \quad -4 \\ n_{R,2} \quad 1 \quad 1 \quad -4 \end{array} \right) \quad (61)$$

$$\left( \begin{array}{l} \text{SG61} \quad a_1 \quad a_2 \quad a_3 \\ \nu \quad 16 \quad 8 \quad -32 \\ n_{\Gamma,1} \quad 4 \quad 4 \quad -12 \\ n_{\Gamma,2} \quad 4 \quad 0 \quad -4 \\ n_{Y,1} \quad 4 \quad 2 \quad -8 \\ n_{Y,2} \quad 4 \quad 2 \quad -8 \\ n_{X,1} \quad 4 \quad 2 \quad -8 \\ n_{X,2} \quad 4 \quad 2 \quad -8 \\ n_{Z,1} \quad 4 \quad 2 \quad -8 \\ n_{Z,2} \quad 4 \quad 2 \quad -8 \\ n_{U,1} \quad 2 \quad 1 \quad -4 \\ n_{U,2} \quad 2 \quad 1 \quad -4 \\ n_{T,1} \quad 2 \quad 1 \quad -4 \\ n_{T,2} \quad 2 \quad 1 \quad -4 \\ n_{S,1} \quad 2 \quad 1 \quad -4 \\ n_{S,2} \quad 2 \quad 1 \quad -4 \\ n_{R,1} \quad 1 \quad 0 \quad 0 \\ n_{R,2} \quad 1 \quad 0 \quad 0 \\ n_{R,3} \quad 1 \quad 0 \quad 0 \\ n_{R,4} \quad 1 \quad 0 \quad 0 \\ n_{R,5} \quad 1 \quad 1 \quad -4 \\ n_{R,6} \quad 1 \quad 1 \quad -4 \\ n_{R,7} \quad 1 \quad 1 \quad -4 \\ n_{R,8} \quad 1 \quad 1 \quad -4 \end{array} \right) \quad (62)$$

$$\left( \begin{array}{l} \text{SG62 } a_1 \quad a_2 \quad a_3 \\ \nu \quad 8 \quad 8 \quad -32 \\ n_{\Gamma,1} \quad 2 \quad 4 \quad -12 \\ n_{\Gamma,2} \quad 2 \quad 0 \quad -4 \\ n_{Y,1} \quad 2 \quad 2 \quad -8 \\ n_{Y,2} \quad 2 \quad 2 \quad -8 \\ n_{X,1} \quad 2 \quad 2 \quad -8 \\ n_{X,2} \quad 2 \quad 2 \quad -8 \\ n_{Z,1} \quad 2 \quad 2 \quad -8 \\ n_{Z,2} \quad 2 \quad 2 \quad -8 \\ n_{U,1} \quad 1 \quad 0 \quad 0 \\ n_{U,2} \quad 1 \quad 2 \quad -8 \\ n_{T,1} \quad 2 \quad 2 \quad -8 \\ n_{T,2} \quad 2 \quad 2 \quad -8 \\ n_{S,1} \quad 1 \quad 1 \quad -4 \\ n_{S,2} \quad 1 \quad 1 \quad -4 \\ n_{R,1} \quad 1 \quad 1 \quad -4 \\ n_{R,2} \quad 1 \quad 1 \quad -4 \end{array} \right) \quad (63)$$

$$\left( \begin{array}{l} \text{SG63 } a_1 \quad a_2 \quad a_3 \quad a_4 \\ \nu \quad 4 \quad -4 \quad 8 \quad -16 \\ n_{\Gamma,1} \quad 1 \quad -2 \quad 4 \quad -8 \\ n_{\Gamma,2} \quad 1 \quad 0 \quad 0 \quad 0 \\ n_{Y,1} \quad 1 \quad -2 \quad 4 \quad -4 \\ n_{Y,2} \quad 1 \quad 0 \quad 0 \quad -4 \\ n_{Z,1} \quad 1 \quad -1 \quad 2 \quad -4 \\ n_{Z,2} \quad 1 \quad -1 \quad 2 \quad -4 \\ n_{T,1} \quad 1 \quad -1 \quad 2 \quad -4 \\ n_{T,2} \quad 1 \quad -1 \quad 2 \quad -4 \\ n_{S,1} \quad 1 \quad 2 \quad -2 \quad 0 \\ n_{S,2} \quad 1 \quad 2 \quad -2 \quad 0 \\ n_{S,3} \quad 1 \quad -4 \quad 6 \quad -8 \\ n_{S,4} \quad 1 \quad -4 \quad 6 \quad -8 \\ n_{R,1} \quad 1 \quad -1 \quad 2 \quad -4 \end{array} \right) \quad (64)$$

$$\left( \begin{array}{l} \text{SG64 } a_1 \quad a_2 \quad a_3 \quad a_4 \\ \nu \quad 8 \quad -12 \quad 16 \quad -16 \\ n_{\Gamma,1} \quad 2 \quad -4 \quad 6 \quad -8 \\ n_{\Gamma,2} \quad 2 \quad -2 \quad 2 \quad 0 \\ n_{Y,1} \quad 2 \quad -4 \quad 6 \quad -4 \\ n_{Y,2} \quad 2 \quad -2 \quad 2 \quad -4 \\ n_{Z,1} \quad 2 \quad -3 \quad 4 \quad -4 \\ n_{Z,2} \quad 2 \quad -3 \quad 4 \quad -4 \\ n_{T,1} \quad 2 \quad -3 \quad 4 \quad -4 \\ n_{T,2} \quad 2 \quad -3 \quad 4 \quad -4 \\ n_{S,1} \quad 2 \quad -3 \quad 4 \quad -4 \\ n_{R,1} \quad 1 \quad 0 \quad 0 \quad 0 \\ n_{R,2} \quad 1 \quad 0 \quad 0 \quad 0 \\ n_{R,3} \quad 1 \quad -3 \quad 4 \quad -4 \\ n_{R,4} \quad 1 \quad -3 \quad 4 \quad -4 \end{array} \right) \quad (65)$$

$$\left( \begin{array}{ccccccc} \text{SG65} & a_1 & a_2 & a_3 & a_4 & a_5 & a_6 & a_7 \\ \nu & 4 & 4 & -8 & 2 & -4 & 8 & -8 \\ n_{\Gamma,1} & 1 & 2 & -4 & 1 & -2 & 4 & -4 \\ n_{\Gamma,2} & 1 & 0 & 0 & 0 & 0 & 0 & 0 \\ n_{Y,1} & 1 & 0 & -2 & 1 & 0 & 2 & -4 \\ n_{Y,2} & 1 & 2 & -2 & 0 & -2 & 2 & 0 \\ n_{Z,1} & 1 & 0 & -1 & 0 & 0 & 2 & -4 \\ n_{Z,2} & 1 & 2 & -3 & 1 & -2 & 2 & 0 \\ n_{T,1} & 1 & 2 & -3 & 0 & -2 & 4 & 0 \\ n_{T,2} & 1 & 0 & -1 & 1 & 0 & 0 & -4 \\ n_{S,1} & 1 & 1 & -1 & 1 & -2 & 0 & 0 \\ n_{S,2} & 1 & 1 & -1 & 1 & -2 & 0 & 0 \\ n_{S,3} & 1 & 1 & -3 & 0 & 0 & 4 & -4 \\ n_{S,4} & 1 & 1 & -3 & 0 & 0 & 4 & -4 \\ n_{R,1} & 1 & 1 & 0 & 0 & 0 & 0 & 0 \\ n_{R,2} & 1 & 1 & 0 & 0 & 0 & 0 & 0 \\ n_{R,3} & 1 & 1 & -4 & 1 & -2 & 4 & -4 \\ n_{R,4} & 1 & 1 & -4 & 1 & -2 & 4 & -4 \end{array} \right) \quad (66)$$

$$\left( \begin{array}{cccccc} \text{SG66} & a_1 & a_2 & a_3 & a_4 & a_5 \\ \nu & 4 & 4 & -12 & 16 & -16 \\ n_{\Gamma,1} & 1 & 2 & -6 & 8 & -8 \\ n_{\Gamma,2} & 1 & 0 & 0 & 0 & 0 \\ n_{Y,1} & 1 & 0 & -2 & 4 & -4 \\ n_{Y,2} & 1 & 2 & -4 & 4 & -4 \\ n_{Z,1} & 1 & 1 & -3 & 4 & -4 \\ n_{Z,2} & 1 & 1 & -3 & 4 & -4 \\ n_{T,1} & 1 & 1 & -3 & 4 & -4 \\ n_{T,2} & 1 & 1 & -3 & 4 & -4 \\ n_{S,1} & 1 & 1 & 0 & 0 & 0 \\ n_{S,2} & 1 & 1 & 0 & 0 & 0 \\ n_{S,3} & 1 & 1 & -6 & 8 & -8 \\ n_{S,4} & 1 & 1 & -6 & 8 & -8 \\ n_{R,1} & 1 & 2 & -5 & 6 & -4 \\ n_{R,2} & 1 & 2 & -5 & 6 & -4 \\ n_{R,3} & 1 & 0 & -1 & 2 & -4 \\ n_{R,4} & 1 & 0 & -1 & 2 & -4 \end{array} \right) \quad (67)$$

$$\left( \begin{array}{ccccc} \text{SG67} & a_1 & a_2 & a_3 & a_4 & a_5 \\ \nu & 4 & 4 & 0 & 0 & 0 \\ n_{\Gamma,1} & 1 & 2 & 0 & 0 & 0 \\ n_{\Gamma,2} & 1 & 0 & 0 & 0 & 0 \\ n_{Y,1} & 1 & 0 & 0 & 2 & 0 \\ n_{Y,2} & 1 & 2 & 0 & -2 & 0 \\ n_{Z,1} & 1 & 0 & 2 & 0 & 0 \\ n_{Z,2} & 1 & 2 & -2 & 0 & 0 \\ n_{T,1} & 1 & 2 & -2 & -2 & 4 \\ n_{T,2} & 1 & 0 & 2 & 2 & -4 \\ n_{S,1} & 1 & 1 & 0 & 0 & 0 \\ n_{R,1} & 1 & 1 & 0 & 0 & 0 \end{array} \right) \quad (68)$$

$$\begin{pmatrix} \text{SG68} & a_1 & a_2 & a_3 \\ \nu & 4 & 8 & 0 \\ n_{\Gamma,1} & 1 & 4 & 0 \\ n_{\Gamma,2} & 1 & 0 & 0 \\ n_{Y,1} & 1 & 0 & 4 \\ n_{Y,2} & 1 & 4 & -4 \\ n_{Z,1} & 1 & 2 & 0 \\ n_{Z,2} & 1 & 2 & 0 \\ n_{T,1} & 1 & 2 & 0 \\ n_{T,2} & 1 & 2 & 0 \\ n_{S,1} & 1 & 2 & 0 \\ n_{R,1} & 1 & 2 & 0 \end{pmatrix} \quad (69)$$

$$\begin{pmatrix} \text{SG69} & a_1 & a_2 & a_3 & a_4 & a_5 & a_6 \\ \nu & 4 & 4 & -6 & 0 & 8 & -8 \\ n_{\Gamma,1} & 1 & 2 & -3 & 0 & 4 & -4 \\ n_{\Gamma,2} & 1 & 0 & 0 & 0 & 0 & 0 \\ n_{Y,1} & 1 & 0 & -1 & 0 & 2 & -4 \\ n_{Y,2} & 1 & 2 & -2 & 0 & 2 & 0 \\ n_{X,1} & 1 & 0 & -1 & 2 & 2 & -4 \\ n_{X,2} & 1 & 2 & -2 & -2 & 2 & 0 \\ n_{Z,1} & 1 & 2 & -3 & -2 & 4 & 0 \\ n_{Z,2} & 1 & 0 & 0 & 2 & 0 & -4 \\ n_{L,1} & 1 & 1 & 0 & 0 & 0 & 0 \\ n_{L,2} & 1 & 1 & -3 & 0 & 4 & -4 \end{pmatrix} \quad (70)$$

$$\begin{pmatrix} \text{SG70} & a_1 & a_2 & a_3 \\ \nu & 4 & 8 & -16 \\ n_{\Gamma,1} & 1 & 4 & -8 \\ n_{\Gamma,2} & 1 & 0 & 0 \\ n_{Y,1} & 1 & 2 & -4 \\ n_{Y,2} & 1 & 2 & -4 \\ n_{X,1} & 1 & 2 & -4 \\ n_{X,2} & 1 & 2 & -4 \\ n_{Z,1} & 1 & 2 & -4 \\ n_{Z,2} & 1 & 2 & -4 \\ n_{L,1} & 1 & 1 & 0 \\ n_{L,2} & 1 & 3 & -8 \end{pmatrix} \quad (71)$$

$$\left( \begin{array}{l} \text{SG71} \quad a_1 \quad a_2 \quad a_3 \quad a_4 \quad a_5 \quad a_6 \\ \nu \quad 4 \quad -10 \quad 2 \quad 2 \quad 8 \quad -24 \\ n_{\Gamma,1} \quad 1 \quad -5 \quad 1 \quad 1 \quad 4 \quad -12 \\ n_{\Gamma,2} \quad 1 \quad 0 \quad 0 \quad 0 \quad 0 \quad 0 \\ n_{X,1} \quad 1 \quad -5 \quad 1 \quad 1 \quad 4 \quad -8 \\ n_{X,2} \quad 1 \quad 0 \quad 0 \quad 0 \quad 0 \quad -4 \\ n_{R,1} \quad 1 \quad -1 \quad 1 \quad 0 \quad 0 \quad -4 \\ n_{R,2} \quad 1 \quad -1 \quad 1 \quad 0 \quad 0 \quad -4 \\ n_{R,3} \quad 1 \quad -4 \quad 0 \quad 1 \quad 4 \quad -8 \\ n_{R,4} \quad 1 \quad -4 \quad 0 \quad 1 \quad 4 \quad -8 \\ n_{S,1} \quad 1 \quad -1 \quad 0 \quad 0 \quad 2 \quad -4 \\ n_{S,2} \quad 1 \quad -1 \quad 0 \quad 0 \quad 2 \quad -4 \\ n_{S,3} \quad 1 \quad -4 \quad 1 \quad 1 \quad 2 \quad -8 \\ n_{S,4} \quad 1 \quad -4 \quad 1 \quad 1 \quad 2 \quad -8 \\ n_{T,1} \quad 1 \quad -1 \quad 0 \quad 1 \quad 0 \quad -4 \\ n_{T,2} \quad 1 \quad -1 \quad 0 \quad 1 \quad 0 \quad -4 \\ n_{T,3} \quad 1 \quad -4 \quad 1 \quad 0 \quad 4 \quad -8 \\ n_{T,4} \quad 1 \quad -4 \quad 1 \quad 0 \quad 4 \quad -8 \\ n_{W,1} \quad 2 \quad -5 \quad 1 \quad 1 \quad 4 \quad -12 \end{array} \right) \quad (72)$$

$$\left( \begin{array}{l} \text{SG72} \quad a_1 \quad a_2 \quad a_3 \quad a_4 \\ \nu \quad 4 \quad -4 \quad 8 \quad -16 \\ n_{\Gamma,1} \quad 1 \quad -2 \quad 4 \quad -8 \\ n_{\Gamma,2} \quad 1 \quad 0 \quad 0 \quad 0 \\ n_{X,1} \quad 1 \quad -2 \quad 4 \quad -4 \\ n_{X,2} \quad 1 \quad 0 \quad 0 \quad -4 \\ n_{R,1} \quad 1 \quad -1 \quad 2 \quad -4 \\ n_{S,1} \quad 1 \quad -1 \quad 2 \quad -4 \\ n_{T,1} \quad 1 \quad 2 \quad -2 \quad 0 \\ n_{T,2} \quad 1 \quad 2 \quad -2 \quad 0 \\ n_{T,3} \quad 1 \quad -4 \quad 6 \quad -8 \\ n_{T,4} \quad 1 \quad -4 \quad 6 \quad -8 \\ n_{W,1} \quad 1 \quad -1 \quad 2 \quad -4 \end{array} \right) \quad (73)$$

$$\left( \begin{array}{l} \text{SG73} \quad a_1 \quad a_2 \quad a_3 \\ \nu \quad 8 \quad 0 \quad 0 \\ n_{\Gamma,1} \quad 2 \quad 2 \quad 0 \\ n_{\Gamma,2} \quad 2 \quad -2 \quad 0 \\ n_{X,1} \quad 2 \quad 2 \quad -4 \\ n_{X,2} \quad 2 \quad -2 \quad 4 \\ n_{R,1} \quad 2 \quad 0 \quad 0 \\ n_{S,1} \quad 2 \quad 0 \quad 0 \\ n_{T,1} \quad 2 \quad 0 \quad 0 \\ n_{W,1} \quad 1 \quad 0 \quad 0 \\ n_{W,2} \quad 1 \quad 0 \quad 0 \\ n_{W,3} \quad 1 \quad 0 \quad 0 \\ n_{W,4} \quad 1 \quad 0 \quad 0 \end{array} \right) \quad (74)$$

$$\left( \begin{array}{cccccc} \text{SG74} & a_1 & a_2 & a_3 & a_4 & a_5 \\ \nu & 4 & 4 & -12 & 16 & -16 \\ n_{\Gamma,1} & 1 & 2 & -6 & 8 & -8 \\ n_{\Gamma,2} & 1 & 0 & 0 & 0 & 0 \\ n_{X,1} & 1 & 2 & -4 & 4 & -4 \\ n_{X,2} & 1 & 0 & -2 & 4 & -4 \\ n_{R,1} & 1 & 1 & -6 & 8 & -8 \\ n_{R,2} & 1 & 1 & -6 & 8 & -8 \\ n_{R,3} & 1 & 1 & 0 & 0 & 0 \\ n_{R,4} & 1 & 1 & 0 & 0 & 0 \\ n_{S,1} & 1 & 0 & -1 & 2 & -4 \\ n_{S,2} & 1 & 0 & -1 & 2 & -4 \\ n_{S,3} & 1 & 2 & -5 & 6 & -4 \\ n_{S,4} & 1 & 2 & -5 & 6 & -4 \\ n_{T,1} & 1 & 1 & -3 & 4 & -4 \\ n_{W,1} & 1 & 1 & -3 & 4 & -4 \\ n_{W,2} & 1 & 1 & -3 & 4 & -4 \\ n_{W,3} & 1 & 1 & -3 & 4 & -4 \\ n_{W,4} & 1 & 1 & -3 & 4 & -4 \end{array} \right) \quad (75)$$

$$\left( \begin{array}{cccc} \text{SG75} & a_1 & a_2 & a_3 \\ \nu & 4 & 2 & 2 \\ n_{\Gamma,1} & 1 & 1 & 1 \\ n_{\Gamma,2} & 1 & 0 & 0 \\ n_{\Gamma,3} & 1 & 0 & 0 \\ n_{\Gamma,4} & 1 & 1 & 1 \\ n_{M,1} & 1 & 0 & 1 \\ n_{M,2} & 1 & 1 & 0 \\ n_{M,3} & 1 & 1 & 0 \\ n_{M,4} & 1 & 0 & 1 \\ n_{Z,1} & 1 & 1 & 1 \\ n_{Z,2} & 1 & 0 & 0 \\ n_{Z,3} & 1 & 0 & 0 \\ n_{Z,4} & 1 & 1 & 1 \\ n_{A,1} & 1 & 0 & 1 \\ n_{A,2} & 1 & 1 & 0 \\ n_{A,3} & 1 & 1 & 0 \\ n_{A,4} & 1 & 0 & 1 \\ n_{R,1} & 2 & 1 & 1 \\ n_{R,2} & 2 & 1 & 1 \\ n_{X,1} & 2 & 1 & 1 \\ n_{X,2} & 2 & 1 & 1 \end{array} \right) \quad (76)$$

$$\left( \begin{array}{ll} \text{SG76} & a_1 \\ \nu & 8 \\ n_{\Gamma,1} & 2 \\ n_{\Gamma,2} & 2 \\ n_{\Gamma,3} & 2 \\ n_{\Gamma,4} & 2 \\ n_{M,1} & 2 \\ n_{M,2} & 2 \\ n_{M,3} & 2 \\ n_{M,4} & 2 \\ n_{Z,1} & 1 \\ n_{Z,2} & 2 \\ n_{Z,3} & 1 \\ n_{Z,4} & 2 \\ n_{A,1} & 1 \\ n_{A,2} & 2 \\ n_{A,3} & 1 \\ n_{A,4} & 2 \\ n_{R,1} & 2 \\ n_{R,2} & 2 \\ n_{X,1} & 4 \\ n_{X,2} & 4 \end{array} \right) \quad (77)$$

$$\left( \begin{array}{ll} \text{SG77} & a_1 \\ \nu & 4 \\ n_{\Gamma,1} & 1 \\ n_{\Gamma,2} & 1 \\ n_{\Gamma,3} & 1 \\ n_{\Gamma,4} & 1 \\ n_{M,1} & 1 \\ n_{M,2} & 1 \\ n_{M,3} & 1 \\ n_{M,4} & 1 \\ n_{Z,1} & 1 \\ n_{Z,2} & 1 \\ n_{Z,3} & 1 \\ n_{Z,4} & 1 \\ n_{A,1} & 1 \\ n_{A,2} & 1 \\ n_{A,3} & 1 \\ n_{A,4} & 1 \\ n_{R,1} & 2 \\ n_{R,2} & 2 \\ n_{X,1} & 2 \\ n_{X,2} & 2 \end{array} \right) \quad (78)$$

$$\left( \begin{array}{cc} \text{SG78} & a_1 \\ \nu & 8 \\ n_{\Gamma,1} & 2 \\ n_{\Gamma,2} & 2 \\ n_{\Gamma,3} & 2 \\ n_{\Gamma,4} & 2 \\ n_{M,1} & 2 \\ n_{M,2} & 2 \\ n_{M,3} & 2 \\ n_{M,4} & 2 \\ n_{Z,1} & 1 \\ n_{Z,2} & 2 \\ n_{Z,3} & 1 \\ n_{Z,4} & 2 \\ n_{A,1} & 1 \\ n_{A,2} & 2 \\ n_{A,3} & 1 \\ n_{A,4} & 2 \\ n_{R,1} & 2 \\ n_{R,2} & 2 \\ n_{X,1} & 4 \\ n_{X,2} & 4 \end{array} \right) \quad (79)$$

$$\left( \begin{array}{ccc} \text{SG79} & a_1 & a_2 \\ \nu & 4 & 2 \\ n_{\Gamma,1} & 1 & 1 \\ n_{\Gamma,2} & 1 & 0 \\ n_{\Gamma,3} & 1 & 0 \\ n_{\Gamma,4} & 1 & 1 \\ n_{N,1} & 2 & 1 \\ n_{X,1} & 2 & 1 \\ n_{X,2} & 2 & 1 \\ n_{Z,1} & 1 & 1 \\ n_{Z,2} & 1 & 0 \\ n_{Z,3} & 1 & 0 \\ n_{Z,4} & 1 & 1 \\ n_{P,1} & 2 & 1 \\ n_{P,2} & 2 & 1 \end{array} \right) \quad (80)$$

$$\left( \begin{array}{cc} \text{SG80} & a_1 \\ \nu & 4 \\ n_{\Gamma,1} & 1 \\ n_{\Gamma,2} & 1 \\ n_{\Gamma,3} & 1 \\ n_{\Gamma,4} & 1 \\ n_{N,1} & 2 \\ n_{X,1} & 2 \\ n_{X,2} & 2 \\ n_{Z,1} & 1 \\ n_{Z,2} & 1 \\ n_{Z,3} & 1 \\ n_{Z,4} & 1 \\ n_{P,1} & 2 \\ n_{P,2} & 1 \end{array} \right) \quad (81)$$

$$\left( \begin{array}{cccccc} \text{SG81} & a_1 & a_2 & a_3 & a_4 & a_5 \\ \nu & 4 & 2 & 2 & 2 & -4 \\ n_{\Gamma,1} & 1 & 0 & 0 & 0 & 0 \\ n_{\Gamma,2} & 1 & 1 & 1 & 1 & -2 \\ n_{\Gamma,3} & 1 & 1 & 1 & 1 & -2 \\ n_{\Gamma,4} & 1 & 0 & 0 & 0 & 0 \\ n_{M,1} & 1 & 1 & 1 & 0 & -2 \\ n_{M,2} & 1 & 0 & 0 & 1 & 0 \\ n_{M,3} & 1 & 0 & 0 & 1 & 0 \\ n_{M,4} & 1 & 1 & 1 & 0 & -2 \\ n_{Z,1} & 1 & 1 & 0 & 1 & -2 \\ n_{Z,2} & 1 & 0 & 1 & 0 & 0 \\ n_{Z,3} & 1 & 0 & 1 & 0 & 0 \\ n_{Z,4} & 1 & 1 & 0 & 1 & -2 \\ n_{A,1} & 1 & 0 & 1 & 1 & -2 \\ n_{A,2} & 1 & 1 & 0 & 0 & 0 \\ n_{A,3} & 1 & 1 & 0 & 0 & 0 \\ n_{A,4} & 1 & 0 & 1 & 1 & -2 \\ n_{R,1} & 2 & 1 & 1 & 1 & -2 \\ n_{R,2} & 2 & 1 & 1 & 1 & -2 \\ n_{X,1} & 2 & 1 & 1 & 1 & -2 \\ n_{X,2} & 2 & 1 & 1 & 1 & -2 \end{array} \right) \quad (82)$$

$$\left( \begin{array}{cccccc} \text{SG82} & a_1 & a_2 & a_3 & a_4 & a_5 \\ \nu & 4 & 2 & 2 & 2 & -4 \\ n_{\Gamma,1} & 1 & 0 & 0 & 0 & 0 \\ n_{\Gamma,2} & 1 & 1 & 1 & 1 & -2 \\ n_{\Gamma,3} & 1 & 1 & 1 & 1 & -2 \\ n_{\Gamma,4} & 1 & 0 & 0 & 0 & 0 \\ n_{N,1} & 2 & 1 & 1 & 1 & -2 \\ n_{X,1} & 2 & 1 & 1 & 1 & -2 \\ n_{X,2} & 2 & 1 & 1 & 1 & -2 \\ n_{Z,1} & 1 & 1 & 1 & 0 & -2 \\ n_{Z,2} & 1 & 0 & 0 & 1 & 0 \\ n_{Z,3} & 1 & 0 & 0 & 1 & 0 \\ n_{Z,4} & 1 & 1 & 1 & 0 & -2 \\ n_{P,1} & 1 & 0 & 1 & 1 & -2 \\ n_{P,2} & 1 & 0 & 1 & 0 & 0 \\ n_{P,3} & 1 & 1 & 0 & 0 & 0 \\ n_{P,4} & 1 & 1 & 0 & 1 & -2 \end{array} \right) \quad (83)$$

SG83	$a_1$	$a_2$	$a_3$	$a_4$	$a_5$	$a_6$	$a_7$	$a_8$	$a_9$	$a_{10}$	$a_{11}$	$a_{12}$	$a_{13}$
$\nu$	8	4	4	4	4	2	2	2	-48	2	8	40	0
$n_{\Gamma,1}$	1	1	1	1	1	1	0	1	-14	1	2	12	0
$n_{\Gamma,2}$	1	0	0	1	1	0	1	0	-6	0	2	4	0
$n_{\Gamma,3}$	1	0	0	1	1	0	1	0	-6	0	2	4	0
$n_{\Gamma,4}$	1	1	1	1	1	1	0	1	-14	1	2	12	0
$n_{\Gamma,5}$	1	1	1	0	0	0	0	0	-4	0	0	4	0
$n_{\Gamma,6}$	1	0	0	0	0	0	0	0	0	0	0	0	0
$n_{\Gamma,7}$	1	0	0	0	0	0	0	0	0	0	0	0	0
$n_{\Gamma,8}$	1	1	1	0	0	0	0	0	-4	0	0	4	0
$n_{M,1}$	1	0	1	0	0	0	1	0	-6	1	-2	8	0
$n_{M,2}$	1	1	0	0	0	1	0	1	-6	0	2	4	0
$n_{M,3}$	1	1	0	0	0	1	0	1	-6	0	2	4	0
$n_{M,4}$	1	0	1	0	0	0	1	0	-6	1	-2	8	0
$n_{M,5}$	1	0	1	1	1	0	0	0	-6	0	2	4	0
$n_{M,6}$	1	1	0	1	1	0	0	0	-6	0	2	4	0
$n_{M,7}$	1	1	0	1	1	0	0	0	-6	0	2	4	0
$n_{M,8}$	1	0	1	1	1	0	0	0	-6	0	2	4	0
$n_{Z,1}$	1	1	1	0	1	0	0	1	-5	0	2	4	0
$n_{Z,2}$	1	0	0	0	1	0	0	0	0	0	0	0	0
$n_{Z,3}$	1	0	0	0	1	0	0	0	0	0	0	0	0
$n_{Z,4}$	1	1	1	0	1	0	0	1	-5	0	2	4	0
$n_{Z,5}$	1	1	1	1	0	1	0	0	-13	1	0	12	0
$n_{Z,6}$	1	0	0	1	0	0	1	0	-6	0	2	4	0
$n_{Z,7}$	1	0	0	1	0	0	1	0	-6	0	2	4	0
$n_{Z,8}$	1	1	1	1	0	1	0	0	-13	1	0	12	0
$n_{A,1}$	1	0	1	1	0	0	0	0	-11	0	0	12	-8
$n_{A,2}$	1	1	0	1	0	0	0	1	-6	0	2	4	0
$n_{A,3}$	1	1	0	1	0	0	0	1	-6	0	2	4	0
$n_{A,4}$	1	0	1	1	0	0	0	0	-11	0	0	12	-8
$n_{A,5}$	1	0	1	0	1	0	1	0	-1	1	0	0	8
$n_{A,6}$	1	1	0	0	1	1	0	0	-6	0	2	4	0
$n_{A,7}$	1	1	0	0	1	1	0	0	-6	0	2	4	0
$n_{A,8}$	1	0	1	0	1	0	1	0	-1	1	0	0	8
$n_{R,1}$	2	1	1	1	1	1	1	0	-15	0	4	12	0
$n_{R,2}$	2	1	1	1	1	1	1	0	-15	0	4	12	0
$n_{R,3}$	2	1	1	1	1	0	0	1	-9	1	0	8	0
$n_{R,4}$	2	1	1	1	1	0	0	1	-9	1	0	8	0
$n_{X,1}$	2	1	1	1	1	0	0	0	-8	1	0	8	0
$n_{X,2}$	2	1	1	1	1	0	0	0	-8	1	0	8	0
$n_{X,3}$	2	1	1	1	1	1	1	1	-16	0	4	12	0
$n_{X,4}$	2	1	1	1	1	1	1	1	-16	0	4	12	0

$$\left( \begin{array}{ccccccc} \text{SG84} & a_1 & a_2 & a_3 & a_4 & a_5 & a_6 & a_7 \\ \nu & 8 & 4 & 4 & 4 & -28 & 32 & -32 \\ n_{\Gamma,1} & 1 & 1 & 1 & 1 & -7 & 8 & -8 \\ n_{\Gamma,2} & 1 & 0 & 0 & 1 & -3 & 4 & -4 \\ n_{\Gamma,3} & 1 & 0 & 0 & 1 & -3 & 4 & -4 \\ n_{\Gamma,4} & 1 & 1 & 1 & 1 & -7 & 8 & -8 \\ n_{\Gamma,5} & 1 & 0 & 0 & 0 & 0 & 0 & 0 \\ n_{\Gamma,6} & 1 & 1 & 1 & 0 & -4 & 4 & -4 \\ n_{\Gamma,7} & 1 & 1 & 1 & 0 & -4 & 4 & -4 \\ n_{\Gamma,8} & 1 & 0 & 0 & 0 & 0 & 0 & 0 \\ n_{M,1} & 1 & 0 & 1 & 0 & -3 & 4 & -4 \\ n_{M,2} & 1 & 1 & 0 & 0 & -3 & 4 & -4 \\ n_{M,3} & 1 & 1 & 0 & 0 & -3 & 4 & -4 \\ n_{M,4} & 1 & 0 & 1 & 0 & -3 & 4 & -4 \\ n_{M,5} & 1 & 1 & 0 & 1 & -4 & 4 & -4 \\ n_{M,6} & 1 & 0 & 1 & 1 & -4 & 4 & -4 \\ n_{M,7} & 1 & 0 & 1 & 1 & -4 & 4 & -4 \\ n_{M,8} & 1 & 1 & 0 & 1 & -4 & 4 & -4 \\ n_{Z,1} & 2 & 1 & 1 & 1 & -7 & 8 & -8 \\ n_{Z,2} & 2 & 1 & 1 & 1 & -7 & 8 & -8 \\ n_{A,1} & 2 & 1 & 1 & 1 & -7 & 8 & -8 \\ n_{A,2} & 2 & 1 & 1 & 1 & -7 & 8 & -8 \\ n_{R,1} & 2 & 1 & 1 & 2 & -9 & 10 & -8 \\ n_{R,2} & 2 & 1 & 1 & 2 & -9 & 10 & -8 \\ n_{R,3} & 2 & 1 & 1 & 0 & -5 & 6 & -8 \\ n_{R,4} & 2 & 1 & 1 & 0 & -5 & 6 & -8 \\ n_{X,1} & 2 & 1 & 1 & 1 & -4 & 4 & -4 \\ n_{X,2} & 2 & 1 & 1 & 1 & -4 & 4 & -4 \\ n_{X,3} & 2 & 1 & 1 & 1 & -10 & 12 & -12 \\ n_{X,4} & 2 & 1 & 1 & 1 & -10 & 12 & -12 \end{array} \right) \quad (85)$$

$$\left( \begin{array}{cccccc} \text{SG85} & a_1 & a_2 & a_3 & a_4 & a_5 & a_6 \\ \nu & 8 & 0 & 0 & 4 & 0 & -16 \\ n_{\Gamma,1} & 1 & 0 & 0 & 1 & 0 & -4 \\ n_{\Gamma,2} & 1 & 0 & -2 & 0 & 2 & -4 \\ n_{\Gamma,3} & 1 & 0 & -2 & 0 & 2 & -4 \\ n_{\Gamma,4} & 1 & 0 & 0 & 1 & 0 & -4 \\ n_{\Gamma,5} & 1 & 0 & 1 & 1 & -2 & 0 \\ n_{\Gamma,6} & 1 & 0 & 1 & 0 & 0 & 0 \\ n_{\Gamma,7} & 1 & 0 & 1 & 0 & 0 & 0 \\ n_{\Gamma,8} & 1 & 0 & 1 & 1 & -2 & 0 \\ n_{M,1} & 2 & 0 & 0 & 1 & 0 & -4 \\ n_{M,2} & 2 & 0 & 0 & 1 & 0 & -4 \\ n_{Z,1} & 1 & 1 & 3 & 1 & -4 & 0 \\ n_{Z,2} & 1 & -1 & -1 & 0 & 2 & -4 \\ n_{Z,3} & 1 & -1 & -1 & 0 & 2 & -4 \\ n_{Z,4} & 1 & 1 & 3 & 1 & -4 & 0 \\ n_{Z,5} & 1 & -1 & -2 & 1 & 2 & -4 \\ n_{Z,6} & 1 & 1 & 0 & 0 & 0 & 0 \\ n_{Z,7} & 1 & 1 & 0 & 0 & 0 & 0 \\ n_{Z,8} & 1 & -1 & -2 & 1 & 2 & -4 \\ n_{A,1} & 2 & 0 & 0 & 1 & 0 & -4 \\ n_{A,2} & 2 & 0 & 0 & 1 & 0 & -4 \\ n_{R,1} & 2 & 0 & 0 & 1 & 0 & -4 \\ n_{X,1} & 2 & 0 & 0 & 1 & 0 & -4 \end{array} \right) \quad (86)$$

$$\left( \begin{array}{cccccc} \text{SG86} & a_1 & a_2 & a_3 & a_4 & a_5 \\ \nu & 8 & 0 & -4 & 8 & -16 \\ n_{\Gamma,1} & 1 & 0 & -1 & 2 & -4 \\ n_{\Gamma,2} & 1 & 0 & -2 & 2 & -4 \\ n_{\Gamma,3} & 1 & 0 & -2 & 2 & -4 \\ n_{\Gamma,4} & 1 & 0 & -1 & 2 & -4 \\ n_{\Gamma,5} & 1 & 0 & 0 & 0 & 0 \\ n_{\Gamma,6} & 1 & 0 & 1 & 0 & 0 \\ n_{\Gamma,7} & 1 & 0 & 1 & 0 & 0 \\ n_{\Gamma,8} & 1 & 0 & 0 & 0 & 0 \\ n_{M,1} & 2 & 0 & -1 & 2 & -4 \\ n_{M,2} & 2 & 0 & -1 & 2 & -4 \\ n_{Z,1} & 2 & 0 & -1 & 2 & -4 \\ n_{Z,2} & 2 & 0 & -1 & 2 & -4 \\ n_{A,1} & 1 & 1 & 2 & -2 & 0 \\ n_{A,2} & 1 & -1 & -1 & 2 & -4 \\ n_{A,3} & 1 & -1 & -1 & 2 & -4 \\ n_{A,4} & 1 & 1 & 2 & -2 & 0 \\ n_{A,5} & 1 & -1 & -3 & 4 & -4 \\ n_{A,6} & 1 & 1 & 0 & 0 & 0 \\ n_{A,7} & 1 & 1 & 0 & 0 & 0 \\ n_{A,8} & 1 & -1 & -3 & 4 & -4 \\ n_{R,1} & 2 & 0 & -1 & 2 & -4 \\ n_{X,1} & 2 & 0 & -1 & 2 & -4 \end{array} \right) \quad (87)$$

$$\left( \begin{array}{cccccccccc} \text{SG87} & a_1 & a_2 & a_3 & a_4 & a_5 & a_6 & a_7 & a_8 & a_9 \\ \nu & 8 & -86 & 4 & 4 & 4 & 2 & 2 & 72 & -112 \\ n_{\Gamma,1} & 1 & -17 & 1 & 1 & 1 & 1 & 0 & 14 & -24 \\ n_{\Gamma,2} & 1 & -12 & 0 & 0 & 1 & 0 & 1 & 10 & -16 \\ n_{\Gamma,3} & 1 & -12 & 0 & 0 & 1 & 0 & 1 & 10 & -16 \\ n_{\Gamma,4} & 1 & -17 & 1 & 1 & 1 & 1 & 0 & 14 & -24 \\ n_{\Gamma,5} & 1 & -7 & 1 & 0 & 0 & 0 & 0 & 6 & -8 \\ n_{\Gamma,6} & 1 & -7 & 0 & 1 & 0 & 0 & 0 & 6 & -8 \\ n_{\Gamma,7} & 1 & -7 & 0 & 1 & 0 & 0 & 0 & 6 & -8 \\ n_{\Gamma,8} & 1 & -7 & 1 & 0 & 0 & 0 & 0 & 6 & -8 \\ n_{N,1} & 2 & -18 & 1 & 1 & 1 & 0 & 0 & 16 & -24 \\ n_{N,2} & 2 & -25 & 1 & 1 & 1 & 1 & 1 & 20 & -32 \\ n_{X,1} & 2 & -25 & 1 & 1 & 0 & 1 & 1 & 22 & -32 \\ n_{X,2} & 2 & -25 & 1 & 1 & 0 & 1 & 1 & 22 & -32 \\ n_{X,3} & 2 & -18 & 1 & 1 & 2 & 0 & 0 & 14 & -24 \\ n_{X,4} & 2 & -18 & 1 & 1 & 2 & 0 & 0 & 14 & -24 \\ n_{Z,1} & 1 & -12 & 1 & 0 & 1 & 1 & 0 & 10 & -16 \\ n_{Z,2} & 1 & -13 & 0 & 1 & 1 & 0 & 1 & 10 & -16 \\ n_{Z,3} & 1 & -13 & 0 & 1 & 1 & 0 & 1 & 10 & -16 \\ n_{Z,4} & 1 & -12 & 1 & 0 & 1 & 1 & 0 & 10 & -16 \\ n_{Z,5} & 1 & -12 & 1 & 1 & 0 & 0 & 0 & 10 & -16 \\ n_{Z,6} & 1 & -6 & 0 & 0 & 0 & 0 & 0 & 6 & -8 \\ n_{Z,7} & 1 & -6 & 0 & 0 & 0 & 0 & 0 & 6 & -8 \\ n_{Z,8} & 1 & -12 & 1 & 1 & 0 & 0 & 0 & 10 & -16 \\ n_{P,1} & 2 & -18 & 1 & 1 & 1 & 1 & 0 & 14 & -24 \\ n_{P,2} & 2 & -25 & 1 & 1 & 1 & 0 & 1 & 22 & -32 \\ n_{P,3} & 2 & -25 & 1 & 1 & 1 & 0 & 1 & 22 & -32 \\ n_{P,4} & 2 & -18 & 1 & 1 & 1 & 1 & 0 & 14 & -24 \end{array} \right) \quad (88)$$

$$\left( \begin{array}{cccccc} \text{SG88} & a_1 & a_2 & a_3 & a_4 & a_5 \\ \nu & 8 & 8 & -8 & 4 & -16 \\ n_{\Gamma,1} & 1 & 2 & -2 & 1 & -4 \\ n_{\Gamma,2} & 1 & 2 & -2 & 0 & -4 \\ n_{\Gamma,3} & 1 & 2 & -2 & 0 & -4 \\ n_{\Gamma,4} & 1 & 2 & -2 & 1 & -4 \\ n_{\Gamma,5} & 1 & 0 & 0 & 0 & 0 \\ n_{\Gamma,6} & 1 & 0 & 0 & 1 & 0 \\ n_{\Gamma,7} & 1 & 0 & 0 & 1 & 0 \\ n_{\Gamma,8} & 1 & 0 & 0 & 0 & 0 \\ n_{N,1} & 2 & 1 & -1 & 1 & -4 \\ n_{N,2} & 2 & 3 & -3 & 1 & -4 \\ n_{X,1} & 2 & 2 & -2 & 1 & -4 \\ n_{Z,1} & 2 & 2 & -2 & 1 & -4 \\ n_{Z,2} & 2 & 2 & -2 & 1 & -4 \\ n_{P,1} & 2 & 2 & -2 & 1 & -4 \\ n_{P,2} & 1 & 1 & 0 & 0 & 0 \\ n_{P,3} & 2 & 2 & -2 & 1 & -4 \\ n_{P,4} & 1 & 1 & -2 & 1 & -4 \end{array} \right) \quad (89)$$

$$\left( \begin{array}{cccc} \text{SG89} & a_1 & a_2 & a_3 \\ \nu & 4 & 2 & 2 \\ n_{\Gamma,1} & 1 & 1 & 1 \\ n_{\Gamma,2} & 1 & 0 & 0 \\ n_{M,1} & 1 & 0 & 1 \\ n_{M,2} & 1 & 1 & 0 \\ n_{Z,1} & 1 & 1 & 1 \\ n_{Z,2} & 1 & 0 & 0 \\ n_{A,1} & 1 & 0 & 1 \\ n_{A,2} & 1 & 1 & 0 \\ n_{R,1} & 2 & 1 & 1 \\ n_{X,1} & 2 & 1 & 1 \end{array} \right) \quad (90)$$

$$\left( \begin{array}{cc} \text{SG90} & a_1 & a_2 \\ \nu & 4 & 4 \\ n_{\Gamma,1} & 1 & 2 \\ n_{\Gamma,2} & 1 & 0 \\ n_{M,1} & 1 & 1 \\ n_{M,2} & 1 & 1 \\ n_{Z,1} & 1 & 2 \\ n_{Z,2} & 1 & 0 \\ n_{A,1} & 1 & 1 \\ n_{A,2} & 1 & 1 \\ n_{R,1} & 1 & 1 \\ n_{R,2} & 1 & 1 \\ n_{R,3} & 1 & 1 \\ n_{R,4} & 1 & 1 \\ n_{X,1} & 1 & 1 \\ n_{X,2} & 1 & 1 \\ n_{X,3} & 1 & 1 \\ n_{X,4} & 1 & 1 \end{array} \right) \quad (91)$$

$$\left( \begin{array}{cc} \text{SG91} & a_1 \\ \nu & 8 \\ n_{\Gamma,1} & 2 \\ n_{\Gamma,2} & 2 \\ n_{M,1} & 2 \\ n_{M,2} & 2 \\ n_{Z,1} & 1 \\ n_{Z,2} & 1 \\ n_{Z,3} & 1 \\ n_{Z,4} & 1 \\ n_{Z,5} & 2 \\ n_{A,1} & 1 \\ n_{A,2} & 1 \\ n_{A,3} & 1 \\ n_{A,4} & 1 \\ n_{A,5} & 2 \\ n_{R,1} & 2 \\ n_{R,2} & 2 \\ n_{R,3} & 2 \\ n_{R,4} & 2 \\ n_{X,1} & 4 \end{array} \right) \quad (92)$$

$$\left( \begin{array}{cc} \text{SG92} & a_1 \\ \nu & 8 \\ n_{\Gamma,1} & 2 \\ n_{\Gamma,2} & 2 \\ n_{M,1} & 2 \\ n_{M,2} & 2 \\ n_{Z,1} & 1 \\ n_{Z,2} & 1 \\ n_{Z,3} & 1 \\ n_{Z,4} & 1 \\ n_{Z,5} & 2 \\ n_{A,1} & 1 \\ n_{A,2} & 1 \\ n_{A,3} & 1 \\ n_{A,4} & 1 \\ n_{A,5} & 1 \\ n_{R,1} & 2 \\ n_{X,1} & 2 \\ n_{X,2} & 2 \\ n_{X,3} & 2 \\ n_{X,4} & 2 \end{array} \right) \quad (93)$$

$$\left( \begin{array}{cc} \text{SG93} & a_1 \\ \nu & 4 \\ n_{\Gamma,1} & 1 \\ n_{\Gamma,2} & 1 \\ n_{M,1} & 1 \\ n_{M,2} & 1 \\ n_{Z,1} & 1 \\ n_{Z,2} & 1 \\ n_{A,1} & 1 \\ n_{A,2} & 1 \\ n_{R,1} & 2 \\ n_{X,1} & 2 \end{array} \right) \quad (94)$$

$$\left( \begin{array}{cc} \text{SG94} & a_1 \\ \nu & 4 \\ n_{\Gamma,1} & 1 \\ n_{\Gamma,2} & 1 \\ n_{M,1} & 1 \\ n_{M,2} & 1 \\ n_{Z,1} & 1 \\ n_{Z,2} & 1 \\ n_{A,1} & 1 \\ n_{A,2} & 1 \\ n_{R,1} & 1 \\ n_{R,2} & 1 \\ n_{R,3} & 1 \\ n_{R,4} & 1 \\ n_{X,1} & 1 \\ n_{X,2} & 1 \\ n_{X,3} & 1 \\ n_{X,4} & 1 \end{array} \right) \quad (95)$$

$$\left( \begin{array}{cc} \text{SG95} & a_1 \\ \nu & 8 \\ n_{\Gamma,1} & 2 \\ n_{\Gamma,2} & 2 \\ n_{M,1} & 2 \\ n_{M,2} & 2 \\ n_{Z,1} & 1 \\ n_{Z,2} & 1 \\ n_{Z,3} & 1 \\ n_{Z,4} & 1 \\ n_{Z,5} & 2 \\ n_{A,1} & 1 \\ n_{A,2} & 1 \\ n_{A,3} & 1 \\ n_{A,4} & 1 \\ n_{A,5} & 2 \\ n_{R,1} & 2 \\ n_{R,2} & 2 \\ n_{R,3} & 2 \\ n_{R,4} & 2 \\ n_{X,1} & 4 \end{array} \right) \quad (96)$$

$$\left( \begin{array}{cc} \text{SG96} & a_1 \\ \nu & 8 \\ n_{\Gamma,1} & 2 \\ n_{\Gamma,2} & 2 \\ n_{M,1} & 2 \\ n_{M,2} & 2 \\ n_{Z,1} & 1 \\ n_{Z,2} & 1 \\ n_{Z,3} & 1 \\ n_{Z,4} & 1 \\ n_{Z,5} & 2 \\ n_{A,1} & 1 \\ n_{A,2} & 1 \\ n_{A,3} & 1 \\ n_{A,4} & 1 \\ n_{A,5} & 1 \\ n_{R,1} & 2 \\ n_{X,1} & 2 \\ n_{X,2} & 2 \\ n_{X,3} & 2 \\ n_{X,4} & 2 \end{array} \right) \quad (97)$$

$$\left( \begin{array}{ccc} \text{SG97} & a_1 & a_2 \\ \nu & 4 & 2 \\ n_{\Gamma,1} & 1 & 1 \\ n_{\Gamma,2} & 1 & 0 \\ n_{N,1} & 2 & 1 \\ n_{N,2} & 2 & 1 \\ n_{X,1} & 2 & 1 \\ n_{Z,1} & 1 & 1 \\ n_{Z,2} & 1 & 0 \\ n_{P,1} & 2 & 1 \end{array} \right) \quad (98)$$

$$\left( \begin{array}{cc} \text{SG98} & a_1 \\ \nu & 4 \\ n_{\Gamma,1} & 1 \\ n_{\Gamma,2} & 1 \\ n_{N,1} & 2 \\ n_{N,2} & 2 \\ n_{X,1} & 2 \\ n_{Z,1} & 1 \\ n_{Z,2} & 1 \\ n_{P,1} & 1 \\ n_{P,2} & 1 \\ n_{P,3} & 1 \\ n_{P,4} & 1 \end{array} \right) \quad (99)$$

$$\begin{pmatrix} \text{SG99} & a_1 & a_2 & a_3 \\ \nu & 4 & 2 & 2 \\ n_{\Gamma,1} & 1 & 1 & 1 \\ n_{\Gamma,2} & 1 & 0 & 0 \\ n_{M,1} & 1 & 0 & 1 \\ n_{M,2} & 1 & 1 & 0 \\ n_{Z,1} & 1 & 1 & 1 \\ n_{Z,2} & 1 & 0 & 0 \\ n_{A,1} & 1 & 0 & 1 \\ n_{A,2} & 1 & 1 & 0 \\ n_{R,1} & 2 & 1 & 1 \\ n_{X,1} & 2 & 1 & 1 \end{pmatrix} \quad (100)$$

$$\begin{pmatrix} \text{SG100} & a_1 & a_2 \\ \nu & 4 & 4 \\ n_{\Gamma,1} & 1 & 2 \\ n_{\Gamma,2} & 1 & 0 \\ n_{M,1} & 1 & 1 \\ n_{M,2} & 1 & 1 \\ n_{Z,1} & 1 & 2 \\ n_{Z,2} & 1 & 0 \\ n_{A,1} & 1 & 1 \\ n_{A,2} & 1 & 1 \\ n_{R,1} & 1 & 1 \\ n_{R,2} & 1 & 1 \\ n_{R,3} & 1 & 1 \\ n_{R,4} & 1 & 1 \\ n_{X,1} & 1 & 1 \\ n_{X,2} & 1 & 1 \\ n_{X,3} & 1 & 1 \\ n_{X,4} & 1 & 1 \end{pmatrix} \quad (101)$$

$$\begin{pmatrix} \text{SG101} & a_1 \\ \nu & 4 \\ n_{\Gamma,1} & 1 \\ n_{\Gamma,2} & 1 \\ n_{M,1} & 1 \\ n_{M,2} & 1 \\ n_{Z,1} & 1 \\ n_{Z,2} & 1 \\ n_{A,1} & 1 \\ n_{A,2} & 1 \\ n_{R,1} & 1 \\ n_{X,1} & 2 \end{pmatrix} \quad (102)$$

$$\begin{pmatrix} \text{SG102} & a_1 \\ \nu & 4 \\ n_{\Gamma,1} & 1 \\ n_{\Gamma,2} & 1 \\ n_{M,1} & 1 \\ n_{M,2} & 1 \\ n_{Z,1} & 1 \\ n_{Z,2} & 1 \\ n_{A,1} & 1 \\ n_{A,2} & 1 \\ n_{R,1} & 1 \\ n_{R,2} & 1 \\ n_{R,3} & 1 \\ n_{R,4} & 1 \\ n_{X,1} & 1 \\ n_{X,2} & 1 \\ n_{X,3} & 1 \\ n_{X,4} & 1 \end{pmatrix} \quad (103)$$

$$\begin{pmatrix} \text{SG103} & a_1 & a_2 & a_3 \\ \nu & 8 & 4 & 4 \\ n_{\Gamma,1} & 2 & 2 & 2 \\ n_{\Gamma,2} & 2 & 0 & 0 \\ n_{M,1} & 2 & 0 & 2 \\ n_{M,2} & 2 & 2 & 0 \\ n_{Z,1} & 1 & 1 & 1 \\ n_{Z,2} & 1 & 0 & 0 \\ n_{A,1} & 1 & 0 & 1 \\ n_{A,2} & 1 & 1 & 0 \\ n_{R,1} & 2 & 1 & 1 \\ n_{X,1} & 4 & 2 & 2 \end{pmatrix} \quad (104)$$

$$\begin{pmatrix} \text{SG104} & a_1 & a_2 \\ \nu & 8 & 4 \\ n_{\Gamma,1} & 2 & 2 \\ n_{\Gamma,2} & 2 & 0 \\ n_{M,1} & 2 & 1 \\ n_{M,2} & 2 & 1 \\ n_{Z,1} & 1 & 1 \\ n_{Z,2} & 1 & 0 \\ n_{A,1} & 2 & 1 \\ n_{A,2} & 2 & 1 \\ n_{R,1} & 2 & 1 \\ n_{R,2} & 2 & 1 \\ n_{R,3} & 2 & 1 \\ n_{R,4} & 2 & 1 \\ n_{X,1} & 2 & 1 \\ n_{X,2} & 2 & 1 \\ n_{X,3} & 2 & 1 \\ n_{X,4} & 2 & 1 \end{pmatrix} \quad (105)$$

$$\begin{pmatrix} \text{SG105} & a_1 \\ \nu & 4 \\ n_{\Gamma,1} & 1 \\ n_{\Gamma,2} & 1 \\ n_{M,1} & 1 \\ n_{M,2} & 1 \\ n_{Z,1} & 1 \\ n_{Z,2} & 1 \\ n_{A,1} & 1 \\ n_{A,2} & 1 \\ n_{R,1} & 2 \\ n_{X,1} & 2 \end{pmatrix} \quad (106)$$

$$\begin{pmatrix} \text{SG106} & a_1 \\ \nu & 8 \\ n_{\Gamma,1} & 2 \\ n_{\Gamma,2} & 2 \\ n_{M,1} & 2 \\ n_{M,2} & 2 \\ n_{Z,1} & 2 \\ n_{Z,2} & 2 \\ n_{A,1} & 1 \\ n_{A,2} & 1 \\ n_{R,1} & 2 \\ n_{R,2} & 2 \\ n_{R,3} & 2 \\ n_{R,4} & 2 \\ n_{X,1} & 2 \\ n_{X,2} & 2 \\ n_{X,3} & 2 \\ n_{X,4} & 2 \end{pmatrix} \quad (107)$$

$$\begin{pmatrix} \text{SG107} & a_1 & a_2 \\ \nu & 4 & 2 \\ n_{\Gamma,1} & 1 & 1 \\ n_{\Gamma,2} & 1 & 0 \\ n_{N,1} & 2 & 1 \\ n_{N,2} & 2 & 1 \\ n_{X,1} & 2 & 1 \\ n_{Z,1} & 1 & 1 \\ n_{Z,2} & 1 & 0 \\ n_{P,1} & 2 & 1 \end{pmatrix} \quad (108)$$

$$\begin{pmatrix} \text{SG108} & a_1 & a_2 \\ \nu & 4 & 4 \\ n_{\Gamma,1} & 1 & 2 \\ n_{\Gamma,2} & 1 & 0 \\ n_{N,1} & 1 & 1 \\ n_{N,2} & 1 & 1 \\ n_{X,1} & 2 & 2 \\ n_{Z,1} & 1 & 2 \\ n_{Z,2} & 1 & 0 \\ n_{P,1} & 1 & 1 \end{pmatrix} \quad (109)$$

$$\begin{pmatrix} \text{SG109} & a_1 \\ \nu & 4 \\ n_{\Gamma,1} & 1 \\ n_{\Gamma,2} & 1 \\ n_{N,1} & 2 \\ n_{N,2} & 2 \\ n_{X,1} & 1 \\ n_{X,2} & 1 \\ n_{X,3} & 1 \\ n_{X,4} & 1 \\ n_{Z,1} & 1 \\ n_{Z,2} & 1 \\ n_{P,1} & 1 \\ n_{P,2} & 1 \\ n_{P,3} & 1 \\ n_{P,4} & 1 \end{pmatrix} \quad (110)$$

$$\begin{pmatrix} \text{SG110} & a_1 \\ \nu & 8 \\ n_{\Gamma,1} & 2 \\ n_{\Gamma,2} & 2 \\ n_{N,1} & 2 \\ n_{N,2} & 2 \\ n_{X,1} & 2 \\ n_{X,2} & 2 \\ n_{X,3} & 2 \\ n_{X,4} & 2 \\ n_{Z,1} & 2 \\ n_{Z,2} & 2 \\ n_{P,1} & 2 \\ n_{P,2} & 2 \\ n_{P,3} & 1 \\ n_{P,4} & 1 \end{pmatrix} \quad (111)$$

$$\begin{pmatrix} \text{SG111} & a_1 & a_2 & a_3 & a_4 & a_5 \\ \nu & 4 & 2 & 2 & 2 & -4 \\ n_{\Gamma,1} & 1 & 0 & 0 & 0 & 0 \\ n_{\Gamma,2} & 1 & 1 & 1 & 1 & -2 \\ n_{M,1} & 1 & 1 & 0 & 1 & -2 \\ n_{M,2} & 1 & 0 & 1 & 0 & 0 \\ n_{Z,1} & 1 & 0 & 1 & 1 & -2 \\ n_{Z,2} & 1 & 1 & 0 & 0 & 0 \\ n_{A,1} & 1 & 1 & 1 & 0 & -2 \\ n_{A,2} & 1 & 0 & 0 & 1 & 0 \\ n_{R,1} & 2 & 1 & 1 & 1 & -2 \\ n_{X,1} & 2 & 1 & 1 & 1 & -2 \end{pmatrix} \quad (112)$$

$$\left( \begin{array}{cccc} \text{SG112} & a_1 & a_2 & a_3 \\ \nu & 4 & 4 & 0 \\ n_{\Gamma,1} & 1 & 0 & 0 \\ n_{\Gamma,2} & 1 & 2 & 0 \\ n_{M,1} & 1 & 2 & -2 \\ n_{M,2} & 1 & 0 & 2 \\ n_{Z,1} & 1 & 1 & 0 \\ n_{Z,2} & 1 & 1 & 0 \\ n_{A,1} & 1 & 1 & 0 \\ n_{A,2} & 1 & 1 & 0 \\ n_{R,1} & 2 & 2 & 0 \\ n_{X,1} & 2 & 2 & 0 \end{array} \right) \quad (113)$$

$$\left( \begin{array}{cccc} \text{SG113} & a_1 & a_2 & a_3 \\ \nu & 4 & 4 & 0 \\ n_{\Gamma,1} & 1 & 0 & 0 \\ n_{\Gamma,2} & 1 & 2 & 0 \\ n_{M,1} & 1 & 1 & 0 \\ n_{M,2} & 1 & 1 & 0 \\ n_{Z,1} & 1 & 2 & -2 \\ n_{Z,2} & 1 & 0 & 2 \\ n_{A,1} & 1 & 1 & 0 \\ n_{A,2} & 1 & 1 & 0 \\ n_{R,1} & 1 & 1 & 0 \\ n_{R,2} & 1 & 1 & 0 \\ n_{R,3} & 1 & 1 & 0 \\ n_{R,4} & 1 & 1 & 0 \\ n_{X,1} & 1 & 1 & 0 \\ n_{X,2} & 1 & 1 & 0 \\ n_{X,3} & 1 & 1 & 0 \\ n_{X,4} & 1 & 1 & 0 \end{array} \right) \quad (114)$$

$$\left( \begin{array}{cccc} \text{SG114} & a_1 & a_2 & a_3 \\ \nu & 8 & 4 & -8 \\ n_{\Gamma,1} & 2 & 0 & -2 \\ n_{\Gamma,2} & 2 & 2 & -2 \\ n_{M,1} & 2 & 1 & -2 \\ n_{M,2} & 2 & 1 & -2 \\ n_{Z,1} & 2 & 1 & -2 \\ n_{Z,2} & 2 & 1 & -2 \\ n_{A,1} & 1 & 1 & -2 \\ n_{A,2} & 1 & 0 & 0 \\ n_{R,1} & 2 & 1 & -2 \\ n_{R,2} & 2 & 1 & -2 \\ n_{R,3} & 2 & 1 & -2 \\ n_{R,4} & 2 & 1 & -2 \\ n_{X,1} & 2 & 1 & -2 \\ n_{X,2} & 2 & 1 & -2 \\ n_{X,3} & 2 & 1 & -2 \\ n_{X,4} & 2 & 1 & -2 \end{array} \right) \quad (115)$$

$$\left( \begin{array}{cccccc} \text{SG115} & a_1 & a_2 & a_3 & a_4 & a_5 \\ \nu & 4 & 2 & 2 & 2 & -4 \\ n_{\Gamma,1} & 1 & 0 & 0 & 0 & 0 \\ n_{\Gamma,2} & 1 & 1 & 1 & 1 & -2 \\ n_{M,1} & 1 & 0 & 1 & 1 & -2 \\ n_{M,2} & 1 & 1 & 0 & 0 & 0 \\ n_{Z,1} & 1 & 1 & 1 & 0 & -2 \\ n_{Z,2} & 1 & 0 & 0 & 1 & 0 \\ n_{A,1} & 1 & 1 & 0 & 1 & -2 \\ n_{A,2} & 1 & 0 & 1 & 0 & 0 \\ n_{R,1} & 2 & 1 & 1 & 1 & -2 \\ n_{X,1} & 2 & 1 & 1 & 1 & -2 \end{array} \right) \quad (116)$$

$$\left( \begin{array}{cccc} \text{SG116} & a_1 & a_2 & a_3 \\ \nu & 4 & 4 & 0 \\ n_{\Gamma,1} & 1 & 0 & 0 \\ n_{\Gamma,2} & 1 & 2 & 0 \\ n_{M,1} & 1 & 2 & -2 \\ n_{M,2} & 1 & 0 & 2 \\ n_{Z,1} & 1 & 1 & 0 \\ n_{Z,2} & 1 & 1 & 0 \\ n_{A,1} & 1 & 1 & 0 \\ n_{A,2} & 1 & 1 & 0 \\ n_{R,1} & 1 & 1 & 0 \\ n_{X,1} & 2 & 2 & 0 \end{array} \right) \quad (117)$$

$$\left( \begin{array}{cccc} \text{SG117} & a_1 & a_2 & a_3 \\ \nu & 4 & 4 & 0 \\ n_{\Gamma,1} & 1 & 0 & 0 \\ n_{\Gamma,2} & 1 & 2 & 0 \\ n_{M,1} & 1 & 1 & 0 \\ n_{M,2} & 1 & 1 & 0 \\ n_{Z,1} & 1 & 2 & -2 \\ n_{Z,2} & 1 & 0 & 2 \\ n_{A,1} & 1 & 1 & 0 \\ n_{A,2} & 1 & 1 & 0 \\ n_{R,1} & 1 & 1 & 0 \\ n_{R,2} & 1 & 1 & 0 \\ n_{R,3} & 1 & 1 & 0 \\ n_{R,4} & 1 & 1 & 0 \\ n_{X,1} & 1 & 1 & 0 \\ n_{X,2} & 1 & 1 & 0 \\ n_{X,3} & 1 & 1 & 0 \\ n_{X,4} & 1 & 1 & 0 \end{array} \right) \quad (118)$$

$$\begin{pmatrix} \text{SG118} & a_1 & a_2 & a_3 \\ \nu & 4 & 4 & 0 \\ n_{\Gamma,1} & 1 & 0 & 0 \\ n_{\Gamma,2} & 1 & 2 & 0 \\ n_{M,1} & 1 & 1 & 0 \\ n_{M,2} & 1 & 1 & 0 \\ n_{Z,1} & 1 & 1 & 0 \\ n_{Z,2} & 1 & 1 & 0 \\ n_{A,1} & 1 & 2 & -2 \\ n_{A,2} & 1 & 0 & 2 \\ n_{R,1} & 1 & 1 & 0 \\ n_{R,2} & 1 & 1 & 0 \\ n_{R,3} & 1 & 1 & 0 \\ n_{R,4} & 1 & 1 & 0 \\ n_{X,1} & 1 & 1 & 0 \\ n_{X,2} & 1 & 1 & 0 \\ n_{X,3} & 1 & 1 & 0 \\ n_{X,4} & 1 & 1 & 0 \end{pmatrix} \quad (119)$$

$$\begin{pmatrix} \text{SG119} & a_1 & a_2 & a_3 & a_4 & a_5 \\ \nu & 4 & 2 & 2 & 2 & -4 \\ n_{\Gamma,1} & 1 & 0 & 0 & 0 & 0 \\ n_{\Gamma,2} & 1 & 1 & 1 & 1 & -2 \\ n_{N,1} & 2 & 1 & 1 & 1 & -2 \\ n_{N,2} & 2 & 1 & 1 & 1 & -2 \\ n_{X,1} & 2 & 1 & 1 & 1 & -2 \\ n_{Z,1} & 1 & 1 & 1 & 0 & -2 \\ n_{Z,2} & 1 & 0 & 0 & 1 & 0 \\ n_{P,1} & 1 & 0 & 1 & 1 & -2 \\ n_{P,2} & 1 & 0 & 1 & 0 & 0 \\ n_{P,3} & 1 & 1 & 0 & 0 & 0 \\ n_{P,4} & 1 & 1 & 0 & 1 & -2 \end{pmatrix} \quad (120)$$

$$\begin{pmatrix} \text{SG120} & a_1 & a_2 & a_3 \\ \nu & 4 & 4 & 0 \\ n_{\Gamma,1} & 1 & 0 & 0 \\ n_{\Gamma,2} & 1 & 2 & 0 \\ n_{N,1} & 1 & 1 & 0 \\ n_{N,2} & 1 & 1 & 0 \\ n_{X,1} & 2 & 2 & 0 \\ n_{Z,1} & 1 & 2 & -2 \\ n_{Z,2} & 1 & 0 & 2 \\ n_{P,1} & 1 & 1 & 0 \\ n_{P,2} & 1 & 1 & 0 \\ n_{P,3} & 1 & 1 & 0 \\ n_{P,4} & 1 & 1 & 0 \end{pmatrix} \quad (121)$$

$$\left( \begin{array}{ccccc} \text{SG121} & a_1 & a_2 & a_3 & a_4 \\ \nu & 4 & 4 & 2 & -4 \\ n_{\Gamma,1} & 1 & 0 & 0 & 0 \\ n_{\Gamma,2} & 1 & 2 & 1 & -2 \\ n_{N,1} & 2 & 2 & 1 & -2 \\ n_{N,2} & 2 & 2 & 1 & -2 \\ n_{X,1} & 2 & 2 & 1 & -2 \\ n_{Z,1} & 1 & 2 & 0 & -2 \\ n_{Z,2} & 1 & 0 & 1 & 0 \\ n_{P,1} & 1 & 1 & 1 & -2 \\ n_{P,2} & 1 & 1 & 0 & 0 \end{array} \right) \quad (122)$$

$$\left( \begin{array}{ccccc} \text{SG122} & a_1 & a_2 & a_3 \\ \nu & 8 & 4 & -8 \\ n_{\Gamma,1} & 2 & 0 & -2 \\ n_{\Gamma,2} & 2 & 2 & -2 \\ n_{N,1} & 4 & 2 & -4 \\ n_{N,2} & 4 & 2 & -4 \\ n_{X,1} & 2 & 1 & -2 \\ n_{X,2} & 2 & 1 & -2 \\ n_{X,3} & 2 & 1 & -2 \\ n_{X,4} & 2 & 1 & -2 \\ n_{Z,1} & 2 & 1 & -2 \\ n_{Z,2} & 2 & 1 & -2 \\ n_{P,1} & 1 & 1 & -2 \\ n_{P,2} & 1 & 1 & -2 \\ n_{P,3} & 1 & 0 & 0 \\ n_{P,4} & 1 & 0 & 0 \\ n_{P,5} & 2 & 1 & -2 \end{array} \right) \quad (123)$$

$$\left( \begin{array}{ccccccccccccccc} \text{SG123} & a_1 & a_2 & a_3 & a_4 & a_5 & a_6 & a_7 & a_8 & a_9 & a_{10} & a_{11} & a_{12} & a_{13} \\ \nu & 8 & 4 & 4 & 4 & 4 & 2 & 2 & 2 & -48 & 2 & 8 & 40 & 0 \\ n_{\Gamma,1} & 1 & 1 & 1 & 1 & 1 & 1 & 0 & 1 & -14 & 1 & 2 & 12 & 0 \\ n_{\Gamma,2} & 1 & 0 & 0 & 1 & 1 & 0 & 1 & 0 & -6 & 0 & 2 & 4 & 0 \\ n_{\Gamma,3} & 1 & 1 & 1 & 0 & 0 & 0 & 0 & 0 & -4 & 0 & 0 & 4 & 0 \\ n_{\Gamma,4} & 1 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ n_{M,1} & 1 & 0 & 1 & 0 & 0 & 0 & 1 & 0 & -6 & 1 & -2 & 8 & 0 \\ n_{M,2} & 1 & 1 & 0 & 0 & 0 & 1 & 0 & 1 & -6 & 0 & 2 & 4 & 0 \\ n_{M,3} & 1 & 0 & 1 & 1 & 1 & 0 & 0 & 0 & -6 & 0 & 2 & 4 & 0 \\ n_{M,4} & 1 & 1 & 0 & 1 & 1 & 0 & 0 & 0 & -6 & 0 & 2 & 4 & 0 \\ n_{Z,1} & 1 & 1 & 1 & 1 & 0 & 0 & 0 & 1 & -5 & 0 & 2 & 4 & 0 \\ n_{Z,2} & 1 & 0 & 0 & 1 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ n_{Z,3} & 1 & 1 & 1 & 0 & 1 & 1 & 0 & 0 & -13 & 1 & 0 & 12 & 0 \\ n_{Z,4} & 1 & 0 & 0 & 0 & 1 & 0 & 1 & 0 & -6 & 0 & 2 & 4 & 0 \\ n_{A,1} & 1 & 0 & 1 & 0 & 1 & 0 & 0 & 0 & -11 & 0 & 0 & 12 & -8 \\ n_{A,2} & 1 & 1 & 0 & 0 & 1 & 0 & 0 & 1 & -6 & 0 & 2 & 4 & 0 \\ n_{A,3} & 1 & 0 & 1 & 1 & 0 & 0 & 1 & 0 & -1 & 1 & 0 & 0 & 8 \\ n_{A,4} & 1 & 1 & 0 & 1 & 0 & 1 & 0 & 0 & -6 & 0 & 2 & 4 & 0 \\ n_{R,1} & 2 & 1 & 1 & 1 & 1 & 1 & 1 & 0 & -15 & 0 & 4 & 12 & 0 \\ n_{R,2} & 2 & 1 & 1 & 1 & 1 & 0 & 0 & 1 & -9 & 1 & 0 & 8 & 0 \\ n_{X,1} & 2 & 1 & 1 & 1 & 1 & 0 & 0 & 0 & -8 & 1 & 0 & 8 & 0 \\ n_{X,2} & 2 & 1 & 1 & 1 & 1 & 1 & 1 & 1 & -16 & 0 & 4 & 12 & 0 \end{array} \right) \quad (124)$$

$$\left( \begin{array}{ccccccccc} \text{SG124} & a_1 & a_2 & a_3 & a_4 & a_5 & a_6 & a_7 & a_8 \\ \nu & 8 & 4 & 4 & 8 & 4 & -36 & 40 & -32 \\ n_{\Gamma,1} & 1 & 1 & 1 & 2 & 2 & -10 & 12 & -8 \\ n_{\Gamma,2} & 1 & 0 & 0 & 2 & 0 & 0 & 0 & 0 \\ n_{\Gamma,3} & 1 & 1 & 1 & 0 & 0 & -8 & 8 & -8 \\ n_{\Gamma,4} & 1 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ n_{M,1} & 1 & 0 & 1 & 0 & 0 & -12 & 14 & -16 \\ n_{M,2} & 1 & 1 & 0 & 0 & 2 & -2 & 2 & 0 \\ n_{M,3} & 1 & 0 & 1 & 2 & 0 & -2 & 2 & 0 \\ n_{M,4} & 1 & 1 & 0 & 2 & 0 & -2 & 2 & 0 \\ n_{Z,1} & 1 & 1 & 1 & 1 & 1 & -9 & 10 & -8 \\ n_{Z,2} & 1 & 1 & 1 & 1 & 1 & -9 & 10 & -8 \\ n_{Z,3} & 1 & 0 & 0 & 1 & 0 & 0 & 0 & 0 \\ n_{Z,4} & 1 & 0 & 0 & 1 & 0 & 0 & 0 & 0 \\ n_{A,1} & 1 & 0 & 1 & 1 & 0 & -7 & 8 & -8 \\ n_{A,2} & 1 & 0 & 1 & 1 & 0 & -7 & 8 & -8 \\ n_{A,3} & 1 & 1 & 0 & 1 & 1 & -2 & 2 & 0 \\ n_{A,4} & 1 & 1 & 0 & 1 & 1 & -2 & 2 & 0 \\ n_{R,1} & 2 & 1 & 1 & 2 & 1 & -9 & 10 & -8 \\ n_{R,2} & 2 & 1 & 1 & 2 & 1 & -9 & 10 & -8 \\ n_{X,1} & 2 & 1 & 1 & 2 & 0 & -8 & 10 & -8 \\ n_{X,2} & 2 & 1 & 1 & 2 & 2 & -10 & 10 & -8 \end{array} \right) \quad (125)$$

$$\left( \begin{array}{ccccccc} \text{SG125} & a_1 & a_2 & a_3 & a_4 & a_5 & a_6 \\ \nu & 8 & 4 & 0 & -4 & 8 & -16 \\ n_{\Gamma,1} & 1 & 1 & 0 & -1 & 2 & -4 \\ n_{\Gamma,2} & 1 & 0 & 0 & -2 & 2 & -4 \\ n_{\Gamma,3} & 1 & 1 & 0 & 0 & 0 & 0 \\ n_{\Gamma,4} & 1 & 0 & 0 & 1 & 0 & 0 \\ n_{M,1} & 2 & 1 & 0 & -1 & 2 & -4 \\ n_{Z,1} & 1 & 1 & 1 & 2 & -2 & 0 \\ n_{Z,2} & 1 & 0 & -1 & -1 & 2 & -4 \\ n_{Z,3} & 1 & 1 & -1 & -3 & 4 & -4 \\ n_{Z,4} & 1 & 0 & 1 & 0 & 0 & 0 \\ n_{A,1} & 2 & 1 & 0 & -1 & 2 & -4 \\ n_{R,1} & 2 & 1 & 0 & -1 & 2 & -4 \\ n_{R,2} & 2 & 1 & 0 & -1 & 2 & -4 \\ n_{X,1} & 2 & 1 & 0 & -1 & 2 & -4 \\ n_{X,2} & 2 & 1 & 0 & -1 & 2 & -4 \end{array} \right) \quad (126)$$

$$\left( \begin{array}{c|ccccc} \text{SG126} & a_1 & a_2 & a_3 & a_4 \\ \nu & 8 & 8 & 4 & 0 \\ n_{\Gamma,1} & 1 & 2 & 1 & 0 \\ n_{\Gamma,2} & 1 & 0 & 0 & -4 \\ n_{\Gamma,3} & 1 & 0 & 1 & 0 \\ n_{\Gamma,4} & 1 & 2 & 0 & 4 \\ n_{M,1} & 2 & 2 & 1 & 0 \\ n_{Z,1} & 1 & 1 & 1 & 0 \\ n_{Z,2} & 1 & 1 & 1 & 0 \\ n_{Z,3} & 1 & 1 & 0 & 0 \\ n_{Z,4} & 1 & 1 & 0 & 0 \\ n_{A,1} & 2 & 2 & 1 & 0 \\ n_{R,1} & 2 & 2 & 1 & 0 \\ n_{R,2} & 2 & 2 & 1 & 0 \\ n_{X,1} & 2 & 2 & 1 & 0 \\ n_{X,2} & 2 & 2 & 1 & 0 \end{array} \right) \quad (127)$$

$$\left( \begin{array}{c|cccccccc} \text{SG127} & a_1 & a_2 & a_3 & a_4 & a_5 & a_6 & a_7 & a_8 \\ \nu & 8 & 8 & 4 & 4 & 4 & -28 & 32 & 0 \\ n_{\Gamma,1} & 1 & 2 & 1 & 1 & 2 & -10 & 12 & 0 \\ n_{\Gamma,2} & 1 & 0 & 1 & 1 & 0 & 0 & 0 & 0 \\ n_{\Gamma,3} & 1 & 2 & 0 & 0 & 0 & -4 & 4 & 0 \\ n_{\Gamma,4} & 1 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ n_{M,1} & 1 & 1 & 1 & 1 & 0 & -4 & 4 & 0 \\ n_{M,2} & 1 & 1 & 1 & 1 & 0 & -4 & 4 & 0 \\ n_{M,3} & 1 & 1 & 0 & 0 & 1 & -3 & 4 & 0 \\ n_{M,4} & 1 & 1 & 0 & 0 & 1 & -3 & 4 & 0 \\ n_{Z,1} & 1 & 2 & 1 & 0 & 0 & -10 & 12 & -8 \\ n_{Z,2} & 1 & 0 & 1 & 0 & 0 & 0 & 0 & 0 \\ n_{Z,3} & 1 & 2 & 0 & 1 & 2 & -4 & 4 & 8 \\ n_{Z,4} & 1 & 0 & 0 & 1 & 0 & 0 & 0 & 0 \\ n_{A,1} & 1 & 1 & 1 & 0 & 1 & -4 & 4 & 0 \\ n_{A,2} & 1 & 1 & 1 & 0 & 1 & -4 & 4 & 0 \\ n_{A,3} & 1 & 1 & 0 & 1 & 0 & -3 & 4 & 0 \\ n_{A,4} & 1 & 1 & 0 & 1 & 0 & -3 & 4 & 0 \\ n_{R,1} & 2 & 2 & 1 & 1 & 1 & -7 & 8 & 0 \\ n_{R,2} & 2 & 2 & 1 & 1 & 1 & -7 & 8 & 0 \\ n_{X,1} & 2 & 2 & 1 & 1 & 1 & -7 & 8 & 0 \\ n_{X,2} & 2 & 2 & 1 & 1 & 1 & -7 & 8 & 0 \end{array} \right) \quad (128)$$

$$\left( \begin{array}{ccccccc} \text{SG128} & a_1 & a_2 & a_3 & a_4 & a_5 & a_6 & a_7 \\ \nu & 8 & 8 & 8 & 4 & 4 & 4 & -96 \\ n_{\Gamma,1} & 1 & 2 & 2 & 2 & 0 & 2 & -24 \\ n_{\Gamma,2} & 1 & 0 & 2 & 0 & 2 & 0 & -16 \\ n_{\Gamma,3} & 1 & 2 & 0 & 0 & 0 & 0 & -8 \\ n_{\Gamma,4} & 1 & 0 & 0 & 0 & 0 & 0 & 0 \\ n_{M,1} & 1 & 1 & 2 & 0 & 0 & 0 & -8 \\ n_{M,2} & 1 & 1 & 2 & 0 & 0 & 0 & -8 \\ n_{M,3} & 1 & 1 & 0 & 1 & 1 & 1 & -16 \\ n_{M,4} & 1 & 1 & 0 & 1 & 1 & 1 & -16 \\ n_{Z,1} & 1 & 2 & 1 & 1 & 0 & 1 & -16 \\ n_{Z,2} & 1 & 2 & 1 & 1 & 0 & 1 & -16 \\ n_{Z,3} & 1 & 0 & 1 & 0 & 1 & 0 & -8 \\ n_{Z,4} & 1 & 0 & 1 & 0 & 1 & 0 & -8 \\ n_{A,1} & 1 & 1 & 1 & 0 & 1 & 1 & -16 \\ n_{A,2} & 1 & 1 & 1 & 0 & 1 & 1 & -16 \\ n_{A,3} & 1 & 1 & 1 & 1 & 0 & 0 & -8 \\ n_{A,4} & 1 & 1 & 1 & 1 & 0 & 0 & -8 \\ n_{R,1} & 1 & 1 & 1 & 0 & 0 & 1 & -8 \\ n_{R,2} & 1 & 1 & 1 & 0 & 0 & 1 & -8 \\ n_{R,3} & 1 & 1 & 1 & 0 & 0 & 1 & -8 \\ n_{R,4} & 1 & 1 & 1 & 0 & 0 & 1 & -8 \\ n_{R,5} & 1 & 1 & 1 & 1 & 1 & 0 & -16 \\ n_{R,6} & 1 & 1 & 1 & 1 & 1 & 0 & -16 \\ n_{R,7} & 1 & 1 & 1 & 1 & 1 & 0 & -16 \\ n_{R,8} & 1 & 1 & 1 & 1 & 1 & 0 & -16 \\ n_{X,1} & 2 & 2 & 2 & 1 & 1 & 1 & -24 \\ n_{X,2} & 2 & 2 & 2 & 1 & 1 & 1 & -24 \end{array} \right) \quad (129)$$

$$\left( \begin{array}{ccccccc} \text{SG129} & a_1 & a_2 & a_3 & a_4 & a_5 & a_6 \\ \nu & 8 & 0 & 0 & 4 & 0 & -16 \\ n_{\Gamma,1} & 1 & 0 & 0 & 1 & 0 & -4 \\ n_{\Gamma,2} & 1 & 0 & -2 & 0 & 2 & -4 \\ n_{\Gamma,3} & 1 & 0 & 1 & 1 & -2 & 0 \\ n_{\Gamma,4} & 1 & 0 & 1 & 0 & 0 & 0 \\ n_{M,1} & 2 & 0 & 0 & 1 & 0 & -4 \\ n_{Z,1} & 1 & 1 & 3 & 1 & -4 & 0 \\ n_{Z,2} & 1 & -1 & -1 & 0 & 2 & -4 \\ n_{Z,3} & 1 & -1 & -2 & 1 & 2 & -4 \\ n_{Z,4} & 1 & 1 & 0 & 0 & 0 & 0 \\ n_{A,1} & 2 & 0 & 0 & 1 & 0 & -4 \\ n_{R,1} & 2 & 0 & 0 & 1 & 0 & -4 \\ n_{R,2} & 2 & 0 & 0 & 1 & 0 & -4 \\ n_{X,1} & 2 & 0 & 0 & 1 & 0 & -4 \\ n_{X,2} & 2 & 0 & 0 & 1 & 0 & -4 \end{array} \right) \quad (130)$$

$$\left( \begin{array}{cccc} \text{SG130} & a_1 & a_2 & a_3 & a_4 \\ \nu & 8 & 8 & 8 & 0 \\ n_{\Gamma,1} & 1 & 2 & 2 & 0 \\ n_{\Gamma,2} & 1 & 0 & 0 & -4 \\ n_{\Gamma,3} & 1 & 0 & 2 & 0 \\ n_{\Gamma,4} & 1 & 2 & 0 & 4 \\ n_{M,1} & 2 & 2 & 2 & 0 \\ n_{Z,1} & 1 & 1 & 2 & 0 \\ n_{Z,2} & 1 & 1 & 2 & 0 \\ n_{Z,3} & 1 & 1 & 0 & 0 \\ n_{Z,4} & 1 & 1 & 0 & 0 \\ n_{A,1} & 1 & 1 & 1 & 0 \\ n_{R,1} & 1 & 1 & 1 & 0 \\ n_{R,2} & 1 & 1 & 1 & 0 \\ n_{X,1} & 2 & 2 & 2 & 0 \\ n_{X,2} & 2 & 2 & 2 & 0 \end{array} \right) \quad (131)$$

$$\left( \begin{array}{ccccccc} \text{SG131} & a_1 & a_2 & a_3 & a_4 & a_5 & a_6 & a_7 \\ \nu & 8 & 4 & 4 & 4 & -28 & 32 & -32 \\ n_{\Gamma,1} & 1 & 1 & 1 & 1 & -7 & 8 & -8 \\ n_{\Gamma,2} & 1 & 0 & 0 & 1 & -3 & 4 & -4 \\ n_{\Gamma,3} & 1 & 0 & 0 & 0 & 0 & 0 & 0 \\ n_{\Gamma,4} & 1 & 1 & 1 & 0 & -4 & 4 & -4 \\ n_{M,1} & 1 & 0 & 1 & 0 & -3 & 4 & -4 \\ n_{M,2} & 1 & 1 & 0 & 0 & -3 & 4 & -4 \\ n_{M,3} & 1 & 1 & 0 & 1 & -4 & 4 & -4 \\ n_{M,4} & 1 & 0 & 1 & 1 & -4 & 4 & -4 \\ n_{Z,1} & 2 & 1 & 1 & 1 & -7 & 8 & -8 \\ n_{A,1} & 2 & 1 & 1 & 1 & -7 & 8 & -8 \\ n_{R,1} & 2 & 1 & 1 & 2 & -9 & 10 & -8 \\ n_{R,2} & 2 & 1 & 1 & 0 & -5 & 6 & -8 \\ n_{X,1} & 2 & 1 & 1 & 1 & -4 & 4 & -4 \\ n_{X,2} & 2 & 1 & 1 & 1 & -10 & 12 & -12 \end{array} \right) \quad (132)$$

$$\left( \begin{array}{ccccccc} \text{SG132} & a_1 & a_2 & a_3 & a_4 & a_5 & a_6 \\ \nu & 8 & -12 & 4 & 4 & 8 & -32 \\ n_{\Gamma,1} & 1 & -3 & 1 & 1 & 2 & -8 \\ n_{\Gamma,2} & 1 & -1 & 0 & 1 & 0 & -4 \\ n_{\Gamma,3} & 1 & 0 & 0 & 0 & 0 & 0 \\ n_{\Gamma,4} & 1 & -2 & 1 & 0 & 2 & -4 \\ n_{M,1} & 1 & -2 & 0 & 1 & 2 & -4 \\ n_{M,2} & 1 & -2 & 1 & 1 & 0 & -4 \\ n_{M,3} & 1 & -1 & 1 & 0 & 0 & -4 \\ n_{M,4} & 1 & -1 & 0 & 0 & 2 & -4 \\ n_{Z,1} & 2 & -3 & 1 & 1 & 2 & -8 \\ n_{A,1} & 2 & -3 & 1 & 1 & 2 & -8 \\ n_{R,1} & 2 & -3 & 1 & 1 & 2 & -8 \\ n_{R,2} & 2 & -3 & 1 & 1 & 2 & -8 \\ n_{X,1} & 2 & 0 & 1 & 0 & 0 & -4 \\ n_{X,2} & 2 & -6 & 1 & 2 & 4 & -12 \end{array} \right) \quad (133)$$

$$\left( \begin{array}{ccccc} \text{SG133} & a_1 & a_2 & a_3 \\ \nu & 8 & 8 & 0 \\ n_{\Gamma,1} & 1 & 2 & 0 \\ n_{\Gamma,2} & 1 & 0 & -4 \\ n_{\Gamma,3} & 1 & 0 & 0 \\ n_{\Gamma,4} & 1 & 2 & 4 \\ n_{M,1} & 2 & 2 & 0 \\ n_{Z,1} & 2 & 2 & 0 \\ n_{A,1} & 1 & 1 & 0 \\ n_{A,2} & 1 & 1 & 0 \\ n_{A,3} & 1 & 1 & 0 \\ n_{A,4} & 1 & 1 & 0 \\ n_{R,1} & 2 & 2 & 0 \\ n_{R,2} & 2 & 2 & 0 \\ n_{X,1} & 2 & 2 & 0 \\ n_{X,2} & 2 & 2 & 0 \end{array} \right) \quad (134)$$

$$\left( \begin{array}{cccccc} \text{SG134} & a_1 & a_2 & a_3 & a_4 & a_5 \\ \nu & 8 & 0 & -4 & 8 & -16 \\ n_{\Gamma,1} & 1 & 0 & -1 & 2 & -4 \\ n_{\Gamma,2} & 1 & 0 & -2 & 2 & -4 \\ n_{\Gamma,3} & 1 & 0 & 0 & 0 & 0 \\ n_{\Gamma,4} & 1 & 0 & 1 & 0 & 0 \\ n_{M,1} & 2 & 0 & -1 & 2 & -4 \\ n_{Z,1} & 2 & 0 & -1 & 2 & -4 \\ n_{A,1} & 1 & -1 & -1 & 2 & -4 \\ n_{A,2} & 1 & 1 & 2 & -2 & 0 \\ n_{A,3} & 1 & 1 & 0 & 0 & 0 \\ n_{A,4} & 1 & -1 & -3 & 4 & -4 \\ n_{R,1} & 2 & 0 & -1 & 2 & -4 \\ n_{R,2} & 2 & 0 & -1 & 2 & -4 \\ n_{X,1} & 2 & 0 & -1 & 2 & -4 \\ n_{X,2} & 2 & 0 & -1 & 2 & -4 \end{array} \right) \quad (135)$$

$$\left( \begin{array}{ccccc} \text{SG135} & a_1 & a_2 & a_3 & a_4 \\ \nu & 8 & 8 & 8 & -32 \\ n_{\Gamma,1} & 1 & 2 & 2 & -8 \\ n_{\Gamma,2} & 1 & 2 & 0 & -4 \\ n_{\Gamma,3} & 1 & 0 & 0 & 0 \\ n_{\Gamma,4} & 1 & 0 & 2 & -4 \\ n_{M,1} & 1 & 2 & 1 & -8 \\ n_{M,2} & 1 & 2 & 1 & -8 \\ n_{M,3} & 1 & 0 & 1 & 0 \\ n_{M,4} & 1 & 0 & 1 & 0 \\ n_{Z,1} & 2 & 2 & 2 & -8 \\ n_{A,1} & 1 & 1 & 1 & -4 \\ n_{R,1} & 2 & 2 & 2 & -8 \\ n_{R,2} & 2 & 2 & 2 & -8 \\ n_{X,1} & 2 & 2 & 2 & -8 \\ n_{X,2} & 2 & 2 & 2 & -8 \end{array} \right) \quad (136)$$

$$\left( \begin{array}{cccccc} \text{SG136} & a_1 & a_2 & a_3 & a_4 & a_5 \\ \nu & 8 & 8 & 8 & 4 & -48 \\ n_{\Gamma,1} & 1 & 2 & 2 & 1 & -12 \\ n_{\Gamma,2} & 1 & 0 & 2 & 1 & -8 \\ n_{\Gamma,3} & 1 & 0 & 0 & 0 & 0 \\ n_{\Gamma,4} & 1 & 2 & 0 & 0 & -4 \\ n_{M,1} & 1 & 1 & 0 & 1 & -4 \\ n_{M,2} & 1 & 1 & 0 & 1 & -4 \\ n_{M,3} & 1 & 1 & 2 & 0 & -8 \\ n_{M,4} & 1 & 1 & 2 & 0 & -8 \\ n_{Z,1} & 2 & 2 & 2 & 1 & -12 \\ n_{A,1} & 2 & 2 & 2 & 1 & -12 \\ n_{R,1} & 1 & 1 & 1 & 0 & -4 \\ n_{R,2} & 1 & 1 & 1 & 0 & -4 \\ n_{R,3} & 1 & 1 & 1 & 0 & -4 \\ n_{R,4} & 1 & 1 & 1 & 0 & -4 \\ n_{R,5} & 1 & 1 & 1 & 1 & -8 \\ n_{R,6} & 1 & 1 & 1 & 1 & -8 \\ n_{R,7} & 1 & 1 & 1 & 1 & -8 \\ n_{R,8} & 1 & 1 & 1 & 1 & -8 \\ n_{X,1} & 2 & 2 & 2 & 1 & -12 \\ n_{X,2} & 2 & 2 & 2 & 1 & -12 \end{array} \right) \quad (137)$$

$$\left( \begin{array}{ccccc} \text{SG137} & a_1 & a_2 & a_3 & a_4 \\ \nu & 8 & 0 & 4 & -16 \\ n_{\Gamma,1} & 1 & 0 & 1 & -4 \\ n_{\Gamma,2} & 1 & 0 & 0 & -4 \\ n_{\Gamma,3} & 1 & 0 & 0 & 0 \\ n_{\Gamma,4} & 1 & 0 & 1 & 0 \\ n_{M,1} & 2 & 0 & 1 & -4 \\ n_{Z,1} & 2 & 0 & 1 & -4 \\ n_{A,1} & 1 & 1 & 0 & 0 \\ n_{A,2} & 1 & 1 & 0 & 0 \\ n_{A,3} & 1 & -1 & 1 & -4 \\ n_{A,4} & 1 & -1 & 1 & -4 \\ n_{R,1} & 2 & 0 & 1 & -4 \\ n_{R,2} & 2 & 0 & 1 & -4 \\ n_{X,1} & 2 & 0 & 1 & -4 \\ n_{X,2} & 2 & 0 & 1 & -4 \end{array} \right) \quad (138)$$

$$\left( \begin{array}{c|ccccc} \text{SG138} & a_1 & a_2 & a_3 & a_4 \\ \nu & 8 & 8 & 0 & 0 \\ n_{\Gamma,1} & 1 & 2 & 0 & 0 \\ n_{\Gamma,2} & 1 & 2 & -2 & -4 \\ n_{\Gamma,3} & 1 & 0 & 0 & 0 \\ n_{\Gamma,4} & 1 & 0 & 2 & 4 \\ n_{M,1} & 2 & 2 & 0 & 0 \\ n_{Z,1} & 2 & 2 & 0 & 0 \\ n_{A,1} & 1 & 2 & -1 & 0 \\ n_{A,2} & 1 & 2 & -1 & 0 \\ n_{A,3} & 1 & 0 & 1 & 0 \\ n_{A,4} & 1 & 0 & 1 & 0 \\ n_{R,1} & 1 & 1 & 0 & 0 \\ n_{R,2} & 1 & 1 & 0 & 0 \\ n_{X,1} & 2 & 2 & 0 & 0 \\ n_{X,2} & 2 & 2 & 0 & 0 \end{array} \right) \quad (139)$$

$$\left( \begin{array}{c|cccccccc} \text{SG139} & a_1 & a_2 & a_3 & a_4 & a_5 & a_6 & a_7 & a_8 & a_9 \\ \nu & 8 & -86 & 4 & 4 & 4 & 2 & 2 & 72 & -112 \\ n_{\Gamma,1} & 1 & -17 & 1 & 1 & 1 & 1 & 0 & 14 & -24 \\ n_{\Gamma,2} & 1 & -12 & 0 & 0 & 1 & 0 & 1 & 10 & -16 \\ n_{\Gamma,3} & 1 & -7 & 1 & 0 & 0 & 0 & 0 & 6 & -8 \\ n_{\Gamma,4} & 1 & -7 & 0 & 1 & 0 & 0 & 0 & 6 & -8 \\ n_{N,1} & 2 & -18 & 1 & 1 & 1 & 0 & 0 & 16 & -24 \\ n_{N,2} & 2 & -18 & 1 & 1 & 1 & 0 & 0 & 16 & -24 \\ n_{N,3} & 2 & -25 & 1 & 1 & 1 & 1 & 1 & 20 & -32 \\ n_{N,4} & 2 & -25 & 1 & 1 & 1 & 1 & 1 & 20 & -32 \\ n_{X,1} & 2 & -25 & 1 & 1 & 0 & 1 & 1 & 22 & -32 \\ n_{X,2} & 2 & -18 & 1 & 1 & 2 & 0 & 0 & 14 & -24 \\ n_{Z,1} & 1 & -12 & 1 & 0 & 1 & 1 & 0 & 10 & -16 \\ n_{Z,2} & 1 & -13 & 0 & 1 & 1 & 0 & 1 & 10 & -16 \\ n_{Z,3} & 1 & -12 & 1 & 1 & 0 & 0 & 0 & 10 & -16 \\ n_{Z,4} & 1 & -6 & 0 & 0 & 0 & 0 & 0 & 6 & -8 \\ n_{P,1} & 2 & -18 & 1 & 1 & 1 & 1 & 0 & 14 & -24 \\ n_{P,2} & 2 & -25 & 1 & 1 & 1 & 0 & 1 & 22 & -32 \end{array} \right) \quad (140)$$

$$\left( \begin{array}{c|ccccccc} \text{SG140} & a_1 & a_2 & a_3 & a_4 & a_5 & a_6 & a_7 \\ \nu & 8 & 4 & -8 & 4 & 4 & -24 & -32 \\ n_{\Gamma,1} & 1 & 1 & -1 & 1 & 2 & -4 & 0 \\ n_{\Gamma,2} & 1 & 0 & -1 & 1 & 0 & -4 & -8 \\ n_{\Gamma,3} & 1 & 1 & -2 & 0 & 0 & -4 & -8 \\ n_{\Gamma,4} & 1 & 0 & 0 & 0 & 0 & 0 & 0 \\ n_{N,1} & 2 & 1 & -2 & 1 & 1 & -6 & -8 \\ n_{X,1} & 2 & 1 & -2 & 2 & 0 & -6 & -8 \\ n_{X,2} & 2 & 1 & -2 & 0 & 2 & -6 & -8 \\ n_{Z,1} & 1 & 0 & 0 & 1 & 0 & 0 & 0 \\ n_{Z,2} & 1 & 1 & -2 & 1 & 2 & -4 & 0 \\ n_{Z,3} & 1 & 0 & -1 & 0 & 0 & -4 & -8 \\ n_{Z,4} & 1 & 1 & -1 & 0 & 0 & -4 & -8 \\ n_{P,1} & 2 & 1 & -2 & 1 & 1 & -6 & -8 \\ n_{P,2} & 2 & 1 & -2 & 1 & 1 & -6 & -8 \end{array} \right) \quad (141)$$

$$\left( \begin{array}{cccccc} \text{SG141} & a_1 & a_2 & a_3 & a_4 & a_5 \\ \nu & 8 & 8 & -8 & 4 & -16 \\ n_{\Gamma,1} & 1 & 2 & -2 & 1 & -4 \\ n_{\Gamma,2} & 1 & 2 & -2 & 0 & -4 \\ n_{\Gamma,3} & 1 & 0 & 0 & 0 & 0 \\ n_{\Gamma,4} & 1 & 0 & 0 & 1 & 0 \\ n_{N,1} & 2 & 1 & -1 & 1 & -4 \\ n_{N,2} & 2 & 1 & -1 & 1 & -4 \\ n_{N,3} & 2 & 3 & -3 & 1 & -4 \\ n_{N,4} & 2 & 3 & -3 & 1 & -4 \\ n_{X,1} & 2 & 2 & -2 & 1 & -4 \\ n_{X,2} & 2 & 2 & -2 & 1 & -4 \\ n_{Z,1} & 2 & 2 & -2 & 1 & -4 \\ n_{P,1} & 1 & 1 & 0 & 0 & 0 \\ n_{P,2} & 1 & 1 & 0 & 0 & 0 \\ n_{P,3} & 1 & 1 & -2 & 1 & -4 \\ n_{P,4} & 1 & 1 & -2 & 1 & -4 \\ n_{P,5} & 2 & 2 & -2 & 1 & -4 \end{array} \right) \quad (142)$$

$$\left( \begin{array}{cccc} \text{SG142} & a_1 & a_2 & a_3 \\ \nu & 8 & 8 & 0 \\ n_{\Gamma,1} & 1 & 2 & 0 \\ n_{\Gamma,2} & 1 & 0 & -4 \\ n_{\Gamma,3} & 1 & 0 & 0 \\ n_{\Gamma,4} & 1 & 2 & 4 \\ n_{N,1} & 2 & 2 & 0 \\ n_{X,1} & 2 & 2 & 0 \\ n_{X,2} & 2 & 2 & 0 \\ n_{Z,1} & 2 & 2 & 0 \\ n_{P,1} & 1 & 1 & 0 \\ n_{P,2} & 1 & 1 & 0 \\ n_{P,3} & 1 & 1 & 0 \\ n_{P,4} & 1 & 1 & 0 \\ n_{P,5} & 1 & 1 & 0 \end{array} \right) \quad (143)$$

$$\left( \begin{array}{ccccc} \text{SG143} & a_1 & a_2 & a_3 & a_4 \\ \nu & 6 & 2 & 2 & 2 \\ n_{\Gamma,1} & 2 & 1 & 1 & 1 \\ n_{\Gamma,2} & 1 & 0 & 0 & 0 \\ n_{\Gamma,3} & 2 & 1 & 1 & 1 \\ n_{M,1} & 3 & 1 & 1 & 1 \\ n_{A,1} & 2 & 1 & 1 & 1 \\ n_{A,2} & 1 & 0 & 0 & 0 \\ n_{A,3} & 2 & 1 & 1 & 1 \\ n_{L,1} & 3 & 1 & 1 & 1 \\ n_{K,1} & 2 & 0 & 1 & 1 \\ n_{K,2} & 2 & 1 & 1 & 0 \\ n_{K,3} & 2 & 1 & 0 & 1 \\ n_{H,1} & 2 & 0 & 1 & 1 \\ n_{H,2} & 2 & 1 & 1 & 0 \\ n_{H,3} & 2 & 1 & 0 & 1 \end{array} \right) \quad (144)$$

$$\left( \begin{array}{cc} \text{SG144} & a_1 \\ \nu & 6 \\ n_{\Gamma,1} & 2 \\ n_{\Gamma,2} & 1 \\ n_{\Gamma,3} & 2 \\ n_{M,1} & 3 \\ n_{A,1} & 2 \\ n_{A,2} & 1 \\ n_{A,3} & 2 \\ n_{L,1} & 3 \\ n_{K,1} & 2 \\ n_{K,2} & 2 \\ n_{K,3} & 2 \\ n_{H,1} & 2 \\ n_{H,2} & 2 \\ n_{H,3} & 2 \end{array} \right) \quad (145)$$

$$\left( \begin{array}{cc} \text{SG145} & a_1 \\ \nu & 6 \\ n_{\Gamma,1} & 2 \\ n_{\Gamma,2} & 1 \\ n_{\Gamma,3} & 2 \\ n_{M,1} & 3 \\ n_{A,1} & 2 \\ n_{A,2} & 1 \\ n_{A,3} & 2 \\ n_{L,1} & 3 \\ n_{K,1} & 2 \\ n_{K,2} & 2 \\ n_{K,3} & 2 \\ n_{H,1} & 2 \\ n_{H,2} & 2 \\ n_{H,3} & 2 \end{array} \right) \quad (146)$$

$$\left( \begin{array}{ccc} \text{SG146} & a_1 & a_2 \\ \nu & 6 & 2 \\ n_{\Gamma,1} & 2 & 1 \\ n_{\Gamma,2} & 1 & 0 \\ n_{\Gamma,3} & 2 & 1 \\ n_{Z,1} & 2 & 1 \\ n_{Z,2} & 1 & 0 \\ n_{Z,3} & 2 & 1 \\ n_{L,1} & 3 & 1 \\ n_{F,1} & 3 & 1 \end{array} \right) \quad (147)$$

$$\left( \begin{array}{ccccccccc} \text{SG147} & a_1 & a_2 & a_3 & a_4 & a_5 & a_6 & a_7 & a_8 & a_9 \\ \nu & 12 & 6 & 6 & 4 & 4 & 2 & -10 & 12 & -8 \\ n_{\Gamma,1} & 2 & 2 & 2 & 1 & 1 & 1 & -5 & 6 & -4 \\ n_{\Gamma,2} & 1 & 1 & 1 & 0 & 0 & 0 & 0 & 0 & 0 \\ n_{\Gamma,3} & 2 & 2 & 2 & 1 & 1 & 1 & -5 & 6 & -4 \\ n_{\Gamma,4} & 1 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ n_{\Gamma,5} & 2 & 0 & 0 & 1 & 1 & 0 & 0 & 0 & 0 \\ n_{\Gamma,6} & 2 & 0 & 0 & 1 & 1 & 0 & 0 & 0 & 0 \\ n_{M,1} & 3 & 1 & 1 & 1 & 1 & 1 & -3 & 4 & -4 \\ n_{M,2} & 3 & 2 & 2 & 1 & 1 & 0 & -2 & 2 & 0 \\ n_{A,1} & 2 & 0 & 2 & 1 & 1 & 0 & -3 & 4 & -4 \\ n_{A,2} & 1 & 0 & 1 & 0 & 0 & 0 & 0 & 0 & 0 \\ n_{A,3} & 2 & 0 & 2 & 1 & 1 & 0 & -3 & 4 & -4 \\ n_{A,4} & 1 & 1 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ n_{A,5} & 2 & 2 & 0 & 1 & 1 & 1 & -2 & 2 & 0 \\ n_{A,6} & 2 & 2 & 0 & 1 & 1 & 1 & -2 & 2 & 0 \\ n_{L,1} & 3 & 2 & 1 & 1 & 1 & 0 & -1 & 2 & 0 \\ n_{L,2} & 3 & 1 & 2 & 1 & 1 & 1 & -4 & 4 & -4 \\ n_{K,1} & 4 & 2 & 2 & 1 & 2 & 1 & -5 & 6 & -4 \\ n_{K,2} & 2 & 1 & 1 & 1 & 0 & 0 & 0 & 0 & 0 \\ n_{K,3} & 4 & 2 & 2 & 1 & 2 & 1 & -5 & 6 & -4 \\ n_{H,1} & 4 & 2 & 2 & 1 & 2 & 1 & -5 & 6 & -4 \\ n_{H,2} & 2 & 1 & 1 & 1 & 0 & 0 & 0 & 0 & 0 \\ n_{H,3} & 4 & 2 & 2 & 1 & 2 & 1 & -5 & 6 & -4 \end{array} \right) \quad (148)$$

$$\left( \begin{array}{ccccccccc} \text{SG148} & a_1 & a_2 & a_3 & a_4 & a_5 & a_6 & a_7 & a_8 \\ \nu & 12 & 6 & 6 & 4 & 2 & -10 & 12 & -8 \\ n_{\Gamma,1} & 2 & 2 & 2 & 1 & 1 & -5 & 6 & -4 \\ n_{\Gamma,2} & 1 & 1 & 1 & 0 & 0 & 0 & 0 & 0 \\ n_{\Gamma,3} & 2 & 2 & 2 & 1 & 1 & -5 & 6 & -4 \\ n_{\Gamma,4} & 1 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ n_{\Gamma,5} & 2 & 0 & 0 & 1 & 0 & 0 & 0 & 0 \\ n_{\Gamma,6} & 2 & 0 & 0 & 1 & 0 & 0 & 0 & 0 \\ n_{Z,1} & 2 & 2 & 0 & 1 & 0 & -3 & 4 & -4 \\ n_{Z,2} & 1 & 1 & 0 & 0 & 0 & 0 & 0 & 0 \\ n_{Z,3} & 2 & 2 & 0 & 1 & 0 & -3 & 4 & -4 \\ n_{Z,4} & 1 & 0 & 1 & 0 & 0 & 0 & 0 & 0 \\ n_{Z,5} & 2 & 0 & 2 & 1 & 1 & -2 & 2 & 0 \\ n_{Z,6} & 2 & 0 & 2 & 1 & 1 & -2 & 2 & 0 \\ n_{L,1} & 3 & 1 & 2 & 1 & 0 & -1 & 2 & 0 \\ n_{L,2} & 3 & 2 & 1 & 1 & 1 & -4 & 4 & -4 \\ n_{F,1} & 3 & 1 & 1 & 1 & 1 & -3 & 4 & -4 \\ n_{F,2} & 3 & 2 & 2 & 1 & 0 & -2 & 2 & 0 \end{array} \right) \quad (149)$$

$$\left( \begin{array}{ccccc} \text{SG149} & a_1 & a_2 & a_3 & a_4 \\ \nu & 6 & 2 & 2 & 2 \\ n_{\Gamma,1} & 1 & 0 & 0 & 0 \\ n_{\Gamma,2} & 1 & 0 & 0 & 0 \\ n_{\Gamma,3} & 2 & 1 & 1 & 1 \\ n_{M,1} & 3 & 1 & 1 & 1 \\ n_{M,2} & 3 & 1 & 1 & 1 \\ n_{A,1} & 1 & 0 & 0 & 0 \\ n_{A,2} & 1 & 0 & 0 & 0 \\ n_{A,3} & 2 & 1 & 1 & 1 \\ n_{L,1} & 3 & 1 & 1 & 1 \\ n_{L,2} & 3 & 1 & 1 & 1 \\ n_{K,1} & 2 & 0 & 1 & 1 \\ n_{K,2} & 2 & 1 & 1 & 0 \\ n_{K,3} & 2 & 1 & 0 & 1 \\ n_{H,1} & 2 & 0 & 1 & 1 \\ n_{H,2} & 2 & 1 & 1 & 0 \\ n_{H,3} & 2 & 1 & 0 & 1 \end{array} \right) \quad (150)$$

$$\left( \begin{array}{ccccc} \text{SG150} & a_1 & a_2 & a_3 \\ \nu & 6 & 4 & 2 \\ n_{\Gamma,1} & 1 & 0 & 0 \\ n_{\Gamma,2} & 1 & 0 & 0 \\ n_{\Gamma,3} & 2 & 2 & 1 \\ n_{M,1} & 3 & 2 & 1 \\ n_{M,2} & 3 & 2 & 1 \\ n_{A,1} & 1 & 0 & 0 \\ n_{A,2} & 1 & 0 & 0 \\ n_{A,3} & 2 & 2 & 1 \\ n_{L,1} & 3 & 2 & 1 \\ n_{L,2} & 3 & 2 & 1 \\ n_{K,1} & 1 & 1 & 0 \\ n_{K,2} & 1 & 1 & 0 \\ n_{K,3} & 2 & 1 & 1 \\ n_{H,1} & 1 & 1 & 0 \\ n_{H,2} & 1 & 1 & 0 \\ n_{H,3} & 2 & 1 & 1 \end{array} \right) \quad (151)$$

$$\left( \begin{array}{cc} \text{SG151} & a_1 \\ \nu & 6 \\ n_{\Gamma,1} & 1 \\ n_{\Gamma,2} & 1 \\ n_{\Gamma,3} & 2 \\ n_{M,1} & 3 \\ n_{M,2} & 3 \\ n_{A,1} & 1 \\ n_{A,2} & 1 \\ n_{A,3} & 2 \\ n_{L,1} & 3 \\ n_{L,2} & 3 \\ n_{K,1} & 2 \\ n_{K,2} & 2 \\ n_{K,3} & 2 \\ n_{H,1} & 2 \\ n_{H,2} & 2 \\ n_{H,3} & 2 \end{array} \right) \quad (152)$$

$$\left( \begin{array}{cc} \text{SG152} & a_1 \\ \nu & 6 \\ n_{\Gamma,1} & 1 \\ n_{\Gamma,2} & 1 \\ n_{\Gamma,3} & 2 \\ n_{M,1} & 3 \\ n_{M,2} & 3 \\ n_{A,1} & 1 \\ n_{A,2} & 1 \\ n_{A,3} & 2 \\ n_{L,1} & 3 \\ n_{L,2} & 3 \\ n_{K,1} & 1 \\ n_{K,2} & 1 \\ n_{K,3} & 2 \\ n_{H,1} & 1 \\ n_{H,2} & 1 \\ n_{H,3} & 2 \end{array} \right) \quad (153)$$

$$\left( \begin{array}{cc} \text{SG153} & a_1 \\ \nu & 6 \\ n_{\Gamma,1} & 1 \\ n_{\Gamma,2} & 1 \\ n_{\Gamma,3} & 2 \\ n_{M,1} & 3 \\ n_{M,2} & 3 \\ n_{A,1} & 1 \\ n_{A,2} & 1 \\ n_{A,3} & 2 \\ n_{L,1} & 3 \\ n_{L,2} & 3 \\ n_{K,1} & 2 \\ n_{K,2} & 2 \\ n_{K,3} & 2 \\ n_{H,1} & 2 \\ n_{H,2} & 2 \\ n_{H,3} & 2 \end{array} \right) \quad (154)$$

$$\left( \begin{array}{cc} \text{SG154} & a_1 \\ \nu & 6 \\ n_{\Gamma,1} & 1 \\ n_{\Gamma,2} & 1 \\ n_{\Gamma,3} & 2 \\ n_{M,1} & 3 \\ n_{M,2} & 3 \\ n_{A,1} & 1 \\ n_{A,2} & 1 \\ n_{A,3} & 2 \\ n_{L,1} & 3 \\ n_{L,2} & 3 \\ n_{K,1} & 1 \\ n_{K,2} & 1 \\ n_{K,3} & 2 \\ n_{H,1} & 1 \\ n_{H,2} & 1 \\ n_{H,3} & 2 \end{array} \right) \quad (155)$$

$$\left( \begin{array}{ccc} \text{SG155} & a_1 & a_2 \\ \nu & 6 & 2 \\ n_{\Gamma,1} & 1 & 0 \\ n_{\Gamma,2} & 1 & 0 \\ n_{\Gamma,3} & 2 & 1 \\ n_{Z,1} & 1 & 0 \\ n_{Z,2} & 1 & 0 \\ n_{Z,3} & 2 & 1 \\ n_{L,1} & 3 & 1 \\ n_{L,2} & 3 & 1 \\ n_{F,1} & 3 & 1 \\ n_{F,2} & 3 & 1 \end{array} \right) \quad (156)$$

$$\left( \begin{array}{ccccc} \text{SG156} & a_1 & a_2 & a_3 & a_4 \\ \nu & 6 & -2 & -2 & -2 \\ n_{\Gamma,1} & 1 & 0 & 0 & 0 \\ n_{\Gamma,2} & 1 & 0 & 0 & 0 \\ n_{\Gamma,3} & 2 & -1 & -1 & -1 \\ n_{M,1} & 3 & -1 & -1 & -1 \\ n_{M,2} & 3 & -1 & -1 & -1 \\ n_{A,1} & 1 & 0 & 0 & 0 \\ n_{A,2} & 1 & 0 & 0 & 0 \\ n_{A,3} & 2 & -1 & -1 & -1 \\ n_{L,1} & 3 & -1 & -1 & -1 \\ n_{L,2} & 3 & -1 & -1 & -1 \\ n_{K,1} & 2 & 0 & -1 & -1 \\ n_{K,2} & 2 & -1 & -1 & 0 \\ n_{K,3} & 2 & -1 & 0 & -1 \\ n_{H,1} & 2 & 0 & -1 & -1 \\ n_{H,2} & 2 & -1 & -1 & 0 \\ n_{H,3} & 2 & -1 & 0 & -1 \end{array} \right) \quad (157)$$

$$\left( \begin{array}{ccccc} \text{SG157} & a_1 & a_2 & a_3 \\ \nu & 6 & 4 & -2 \\ n_{\Gamma,1} & 1 & 0 & 0 \\ n_{\Gamma,2} & 1 & 0 & 0 \\ n_{\Gamma,3} & 2 & 2 & -1 \\ n_{M,1} & 3 & 2 & -1 \\ n_{M,2} & 3 & 2 & -1 \\ n_{A,1} & 1 & 0 & 0 \\ n_{A,2} & 1 & 0 & 0 \\ n_{A,3} & 2 & 2 & -1 \\ n_{L,1} & 3 & 2 & -1 \\ n_{L,2} & 3 & 2 & -1 \\ n_{K,1} & 1 & 1 & 0 \\ n_{K,2} & 1 & 1 & 0 \\ n_{K,3} & 2 & 1 & -1 \\ n_{H,1} & 1 & 1 & 0 \\ n_{H,2} & 1 & 1 & 0 \\ n_{H,3} & 2 & 1 & -1 \end{array} \right) \quad (158)$$

$$\left( \begin{array}{l} \text{SG158} \quad a_1 \quad a_2 \quad a_3 \quad a_4 \\ \nu \quad 12 \quad 4 \quad 4 \quad 4 \\ n_{\Gamma,1} \quad 2 \quad 0 \quad 0 \quad 0 \\ n_{\Gamma,2} \quad 2 \quad 0 \quad 0 \quad 0 \\ n_{\Gamma,3} \quad 4 \quad 2 \quad 2 \quad 2 \\ n_{M,1} \quad 6 \quad 2 \quad 2 \quad 2 \\ n_{M,2} \quad 6 \quad 2 \quad 2 \quad 2 \\ n_{A,1} \quad 1 \quad 0 \quad 0 \quad 0 \\ n_{A,2} \quad 1 \quad 0 \quad 0 \quad 0 \\ n_{A,3} \quad 2 \quad 1 \quad 1 \quad 1 \\ n_{L,1} \quad 3 \quad 1 \quad 1 \quad 1 \\ n_{L,2} \quad 3 \quad 1 \quad 1 \quad 1 \\ n_{K,1} \quad 4 \quad 0 \quad 2 \quad 2 \\ n_{K,2} \quad 4 \quad 2 \quad 2 \quad 0 \\ n_{K,3} \quad 4 \quad 2 \quad 0 \quad 2 \\ n_{H,1} \quad 2 \quad 0 \quad 1 \quad 1 \\ n_{H,2} \quad 2 \quad 1 \quad 1 \quad 0 \\ n_{H,3} \quad 2 \quad 1 \quad 0 \quad 1 \end{array} \right) \quad (159)$$

$$\left( \begin{array}{l} \text{SG159} \quad a_1 \quad a_2 \quad a_3 \\ \nu \quad 12 \quad 4 \quad 4 \\ n_{\Gamma,1} \quad 2 \quad 0 \quad 0 \\ n_{\Gamma,2} \quad 2 \quad 0 \quad 0 \\ n_{\Gamma,3} \quad 4 \quad 2 \quad 2 \\ n_{M,1} \quad 6 \quad 2 \quad 2 \\ n_{M,2} \quad 6 \quad 2 \quad 2 \\ n_{A,1} \quad 1 \quad 0 \quad 0 \\ n_{A,2} \quad 1 \quad 0 \quad 0 \\ n_{A,3} \quad 2 \quad 1 \quad 1 \\ n_{L,1} \quad 3 \quad 1 \quad 1 \\ n_{L,2} \quad 3 \quad 1 \quad 1 \\ n_{K,1} \quad 2 \quad 1 \quad 0 \\ n_{K,2} \quad 2 \quad 1 \quad 0 \\ n_{K,3} \quad 4 \quad 1 \quad 2 \\ n_{H,1} \quad 2 \quad 1 \quad 0 \\ n_{H,2} \quad 2 \quad 1 \quad 0 \\ n_{H,3} \quad 4 \quad 1 \quad 2 \end{array} \right) \quad (160)$$

$$\left( \begin{array}{l} \text{SG160} \quad a_1 \quad a_2 \\ \nu \quad 6 \quad -2 \\ n_{\Gamma,1} \quad 1 \quad 0 \\ n_{\Gamma,2} \quad 1 \quad 0 \\ n_{\Gamma,3} \quad 2 \quad -1 \\ n_{Z,1} \quad 1 \quad 0 \\ n_{Z,2} \quad 1 \quad 0 \\ n_{Z,3} \quad 2 \quad -1 \\ n_{L,1} \quad 3 \quad -1 \\ n_{L,2} \quad 3 \quad -1 \\ n_{F,1} \quad 3 \quad -1 \\ n_{F,2} \quad 3 \quad -1 \end{array} \right) \quad (161)$$

$$\left( \begin{array}{ccc} \text{SG161} & a_1 & a_2 \\ \nu & 12 & 4 \\ n_{\Gamma,1} & 2 & 0 \\ n_{\Gamma,2} & 2 & 0 \\ n_{\Gamma,3} & 4 & 2 \\ n_{Z,1} & 1 & 0 \\ n_{Z,2} & 1 & 0 \\ n_{Z,3} & 2 & 1 \\ n_{L,1} & 3 & 1 \\ n_{L,2} & 3 & 1 \\ n_{F,1} & 6 & 2 \\ n_{F,2} & 6 & 2 \end{array} \right) \quad (162)$$

$$\left( \begin{array}{ccccccccc} \text{SG162} & a_1 & a_2 & a_3 & a_4 & a_5 & a_6 & a_7 & a_8 & a_9 \\ \nu & 12 & 4 & 6 & 6 & -4 & 0 & 2 & -4 & 8 \\ n_{\Gamma,1} & 1 & 0 & 1 & 1 & 0 & 0 & 0 & 0 & 0 \\ n_{\Gamma,2} & 1 & 0 & 1 & 1 & 0 & 0 & 0 & 0 & 0 \\ n_{\Gamma,3} & 2 & 1 & 2 & 2 & -1 & 0 & 1 & -2 & 4 \\ n_{\Gamma,4} & 1 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ n_{\Gamma,5} & 1 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ n_{\Gamma,6} & 2 & 1 & 0 & 0 & -1 & 0 & 0 & 0 & 0 \\ n_{M,1} & 3 & 1 & 1 & 1 & -1 & 0 & 1 & 0 & 0 \\ n_{M,2} & 3 & 1 & 1 & 1 & -1 & 0 & 1 & 0 & 0 \\ n_{M,3} & 3 & 1 & 2 & 2 & -1 & 0 & 0 & -2 & 4 \\ n_{M,4} & 3 & 1 & 2 & 2 & -1 & 0 & 0 & -2 & 4 \\ n_{A,1} & 1 & 0 & 0 & 1 & 0 & 0 & 0 & 0 & 0 \\ n_{A,2} & 1 & 0 & 0 & 1 & 0 & 0 & 0 & 0 & 0 \\ n_{A,3} & 2 & 1 & 0 & 2 & -1 & 1 & 0 & -2 & 4 \\ n_{A,4} & 1 & 0 & 1 & 0 & 0 & 0 & 0 & 0 & 0 \\ n_{A,5} & 1 & 0 & 1 & 0 & 0 & 0 & 0 & 0 & 0 \\ n_{A,6} & 2 & 1 & 2 & 0 & -1 & -1 & 1 & 0 & 0 \\ n_{L,1} & 3 & 1 & 2 & 1 & -1 & 1 & 0 & 0 & 4 \\ n_{L,2} & 3 & 1 & 2 & 1 & -1 & 1 & 0 & 0 & 4 \\ n_{L,3} & 3 & 1 & 1 & 2 & -1 & -1 & 1 & -2 & 0 \\ n_{L,4} & 3 & 1 & 1 & 2 & -1 & -1 & 1 & -2 & 0 \\ n_{K,1} & 2 & 1 & 1 & 1 & 0 & 0 & 0 & 0 & 0 \\ n_{K,2} & 2 & 1 & 1 & 1 & 0 & 0 & 0 & 0 & 0 \\ n_{K,3} & 4 & 1 & 2 & 2 & -2 & 0 & 1 & -2 & 4 \\ n_{H,1} & 2 & 1 & 1 & 1 & 0 & 0 & 0 & 0 & 0 \\ n_{H,2} & 2 & 1 & 1 & 1 & 0 & 0 & 0 & 0 & 0 \\ n_{H,3} & 4 & 1 & 2 & 2 & -2 & 0 & 1 & -2 & 4 \end{array} \right) \quad (163)$$

$$\left( \begin{array}{ccccccc} \text{SG163} & a_1 & a_2 & a_3 & a_4 & a_5 & a_6 \\ \nu & 12 & 12 & 4 & 4 & 4 & -16 \\ n_{\Gamma,1} & 1 & 2 & 0 & 0 & 0 & 0 \\ n_{\Gamma,2} & 1 & 2 & 0 & 0 & 0 & 0 \\ n_{\Gamma,3} & 2 & 4 & 1 & 1 & 2 & -8 \\ n_{\Gamma,4} & 1 & 0 & 0 & 0 & 0 & 0 \\ n_{\Gamma,5} & 1 & 0 & 0 & 0 & 0 & 0 \\ n_{\Gamma,6} & 2 & 0 & 1 & 1 & 0 & 0 \\ n_{M,1} & 3 & 2 & 1 & 1 & 2 & -4 \\ n_{M,2} & 3 & 2 & 1 & 1 & 2 & -4 \\ n_{M,3} & 3 & 4 & 1 & 1 & 0 & -4 \\ n_{M,4} & 3 & 4 & 1 & 1 & 0 & -4 \\ n_{A,1} & 1 & 1 & 0 & 0 & 0 & 0 \\ n_{A,2} & 2 & 2 & 1 & 1 & 1 & -4 \\ n_{A,3} & 2 & 2 & 1 & 1 & 1 & -4 \\ n_{L,1} & 3 & 3 & 1 & 1 & 1 & -4 \\ n_{K,1} & 2 & 2 & 1 & 0 & 0 & 0 \\ n_{K,2} & 2 & 2 & 1 & 0 & 0 & 0 \\ n_{K,3} & 4 & 4 & 1 & 2 & 2 & -8 \\ n_{H,1} & 2 & 2 & 1 & 0 & 0 & 0 \\ n_{H,2} & 2 & 2 & 1 & 0 & 0 & 0 \\ n_{H,3} & 4 & 4 & 1 & 2 & 2 & -8 \end{array} \right) \quad (164)$$

$$\left( \begin{array}{ccccccccc} \text{SG164} & a_1 & a_2 & a_3 & a_4 & a_5 & a_6 & a_7 & a_8 & a_9 \\ \nu & 12 & 6 & 6 & -4 & -4 & 0 & 2 & -4 & 8 \\ n_{\Gamma,1} & 1 & 1 & 1 & 0 & 0 & 0 & 0 & 0 & 0 \\ n_{\Gamma,2} & 1 & 1 & 1 & 0 & 0 & 0 & 0 & 0 & 0 \\ n_{\Gamma,3} & 2 & 2 & 2 & -1 & -1 & 0 & 1 & -2 & 4 \\ n_{\Gamma,4} & 1 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ n_{\Gamma,5} & 1 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ n_{\Gamma,6} & 2 & 0 & 0 & -1 & -1 & 0 & 0 & 0 & 0 \\ n_{M,1} & 3 & 1 & 1 & -1 & -1 & 0 & 1 & 0 & 0 \\ n_{M,2} & 3 & 1 & 1 & -1 & -1 & 0 & 1 & 0 & 0 \\ n_{M,3} & 3 & 2 & 2 & -1 & -1 & 0 & 0 & -2 & 4 \\ n_{M,4} & 3 & 2 & 2 & -1 & -1 & 0 & 0 & -2 & 4 \\ n_{A,1} & 1 & 0 & 1 & 0 & 0 & 0 & 0 & 0 & 0 \\ n_{A,2} & 1 & 0 & 1 & 0 & 0 & 0 & 0 & 0 & 0 \\ n_{A,3} & 2 & 0 & 2 & -1 & -1 & 1 & 0 & -2 & 4 \\ n_{A,4} & 1 & 1 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ n_{A,5} & 1 & 1 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ n_{A,6} & 2 & 2 & 0 & -1 & -1 & -1 & 1 & 0 & 0 \\ n_{L,1} & 3 & 2 & 1 & -1 & -1 & 1 & 0 & 0 & 4 \\ n_{L,2} & 3 & 2 & 1 & -1 & -1 & 1 & 0 & 0 & 4 \\ n_{L,3} & 3 & 1 & 2 & -1 & -1 & -1 & 1 & -2 & 0 \\ n_{L,4} & 3 & 1 & 2 & -1 & -1 & -1 & 1 & -2 & 0 \\ n_{K,1} & 2 & 1 & 1 & -1 & 0 & 0 & 0 & 0 & 0 \\ n_{K,2} & 2 & 1 & 1 & -1 & 0 & 0 & 0 & 0 & 0 \\ n_{K,3} & 4 & 2 & 2 & -1 & -2 & 0 & 1 & -2 & 4 \\ n_{H,1} & 2 & 1 & 1 & -1 & 0 & 0 & 0 & 0 & 0 \\ n_{H,2} & 2 & 1 & 1 & -1 & 0 & 0 & 0 & 0 & 0 \\ n_{H,3} & 4 & 2 & 2 & -1 & -2 & 0 & 1 & -2 & 4 \end{array} \right) \quad (165)$$

$$\left( \begin{array}{ccccccc} \text{SG165} & a_1 & a_2 & a_3 & a_4 & a_5 & a_6 \\ \nu & 12 & 12 & 8 & 4 & 4 & -16 \\ n_{\Gamma,1} & 1 & 2 & 0 & 0 & 0 & 0 \\ n_{\Gamma,2} & 1 & 2 & 0 & 0 & 0 & 0 \\ n_{\Gamma,3} & 2 & 4 & 2 & 1 & 2 & -8 \\ n_{\Gamma,4} & 1 & 0 & 0 & 0 & 0 & 0 \\ n_{\Gamma,5} & 1 & 0 & 0 & 0 & 0 & 0 \\ n_{\Gamma,6} & 2 & 0 & 2 & 1 & 0 & 0 \\ n_{M,1} & 3 & 2 & 2 & 1 & 2 & -4 \\ n_{M,2} & 3 & 2 & 2 & 1 & 2 & -4 \\ n_{M,3} & 3 & 4 & 2 & 1 & 0 & -4 \\ n_{M,4} & 3 & 4 & 2 & 1 & 0 & -4 \\ n_{A,1} & 1 & 1 & 0 & 0 & 0 & 0 \\ n_{A,2} & 2 & 2 & 2 & 1 & 1 & -4 \\ n_{A,3} & 2 & 2 & 2 & 1 & 1 & -4 \\ n_{L,1} & 3 & 3 & 2 & 1 & 1 & -4 \\ n_{K,1} & 2 & 2 & 2 & 0 & 0 & 0 \\ n_{K,2} & 2 & 2 & 2 & 0 & 0 & 0 \\ n_{K,3} & 4 & 4 & 2 & 2 & 2 & -8 \\ n_{H,1} & 1 & 1 & 1 & 0 & 0 & 0 \\ n_{H,2} & 1 & 1 & 1 & 0 & 0 & 0 \\ n_{H,3} & 2 & 2 & 1 & 1 & 1 & -4 \end{array} \right) \quad (166)$$

$$\left( \begin{array}{cccccccc} \text{SG166} & a_1 & a_2 & a_3 & a_4 & a_5 & a_6 & a_7 & a_8 \\ \nu & 12 & 6 & 6 & -4 & 0 & 2 & -4 & 8 \\ n_{\Gamma,1} & 1 & 1 & 1 & 0 & 0 & 0 & 0 & 0 \\ n_{\Gamma,2} & 1 & 1 & 1 & 0 & 0 & 0 & 0 & 0 \\ n_{\Gamma,3} & 2 & 2 & 2 & -1 & 0 & 1 & -2 & 4 \\ n_{\Gamma,4} & 1 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ n_{\Gamma,5} & 1 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ n_{\Gamma,6} & 2 & 0 & 0 & -1 & 0 & 0 & 0 & 0 \\ n_{Z,1} & 1 & 1 & 0 & 0 & 0 & 0 & 0 & 0 \\ n_{Z,2} & 1 & 1 & 0 & 0 & 0 & 0 & 0 & 0 \\ n_{Z,3} & 2 & 2 & 0 & -1 & 1 & 0 & -2 & 4 \\ n_{Z,4} & 1 & 0 & 1 & 0 & 0 & 0 & 0 & 0 \\ n_{Z,5} & 1 & 0 & 1 & 0 & 0 & 0 & 0 & 0 \\ n_{Z,6} & 2 & 0 & 2 & -1 & -1 & 1 & 0 & 0 \\ n_{L,1} & 3 & 1 & 2 & -1 & 1 & 0 & 0 & 4 \\ n_{L,2} & 3 & 1 & 2 & -1 & 1 & 0 & 0 & 4 \\ n_{L,3} & 3 & 2 & 1 & -1 & -1 & 1 & -2 & 0 \\ n_{L,4} & 3 & 2 & 1 & -1 & -1 & 1 & -2 & 0 \\ n_{F,1} & 3 & 1 & 1 & -1 & 0 & 1 & 0 & 0 \\ n_{F,2} & 3 & 1 & 1 & -1 & 0 & 1 & 0 & 0 \\ n_{F,3} & 3 & 2 & 2 & -1 & 0 & 0 & -2 & 4 \\ n_{F,4} & 3 & 2 & 2 & -1 & 0 & 0 & -2 & 4 \end{array} \right) \quad (167)$$

$$\left( \begin{array}{cccccc} \text{SG167} & a_1 & a_2 & a_3 & a_4 & a_5 \\ \nu & 12 & 12 & 4 & 4 & -16 \\ n_{\Gamma,1} & 1 & 2 & 0 & 0 & 0 \\ n_{\Gamma,2} & 1 & 2 & 0 & 0 & 0 \\ n_{\Gamma,3} & 2 & 4 & 1 & 2 & -8 \\ n_{\Gamma,4} & 1 & 0 & 0 & 0 & 0 \\ n_{\Gamma,5} & 1 & 0 & 0 & 0 & 0 \\ n_{\Gamma,6} & 2 & 0 & 1 & 0 & 0 \\ n_{Z,1} & 1 & 1 & 0 & 0 & 0 \\ n_{Z,2} & 2 & 2 & 1 & 1 & -4 \\ n_{Z,3} & 2 & 2 & 1 & 1 & -4 \\ n_{L,1} & 3 & 3 & 1 & 1 & -4 \\ n_{F,1} & 3 & 2 & 1 & 2 & -4 \\ n_{F,2} & 3 & 2 & 1 & 2 & -4 \\ n_{F,3} & 3 & 4 & 1 & 0 & -4 \\ n_{F,4} & 3 & 4 & 1 & 0 & -4 \end{array} \right) \quad (168)$$

$$\left( \begin{array}{ccccc} \text{SG168} & a_1 & a_2 & a_3 & a_4 \\ \nu & 6 & 4 & 2 & 2 \\ n_{\Gamma,1} & 1 & 1 & 1 & 0 \\ n_{\Gamma,2} & 1 & 0 & 0 & 1 \\ n_{\Gamma,3} & 1 & 1 & 0 & 0 \\ n_{\Gamma,4} & 1 & 1 & 0 & 0 \\ n_{\Gamma,5} & 1 & 0 & 0 & 1 \\ n_{\Gamma,6} & 1 & 1 & 1 & 0 \\ n_{M,1} & 3 & 2 & 1 & 1 \\ n_{M,2} & 3 & 2 & 1 & 1 \\ n_{A,1} & 1 & 1 & 1 & 0 \\ n_{A,2} & 1 & 0 & 0 & 1 \\ n_{A,3} & 1 & 1 & 0 & 0 \\ n_{A,4} & 1 & 1 & 0 & 0 \\ n_{A,5} & 1 & 0 & 0 & 1 \\ n_{A,6} & 1 & 1 & 1 & 0 \\ n_{L,1} & 3 & 2 & 1 & 1 \\ n_{L,2} & 3 & 2 & 1 & 1 \\ n_{K,1} & 2 & 1 & 1 & 0 \\ n_{K,2} & 2 & 2 & 0 & 2 \\ n_{K,3} & 2 & 1 & 1 & 0 \\ n_{H,1} & 2 & 1 & 1 & 0 \\ n_{H,2} & 2 & 2 & 0 & 2 \\ n_{H,3} & 2 & 1 & 1 & 0 \end{array} \right) \quad (169)$$

$$\left( \begin{array}{cc} \text{SG169} & a_1 \\ \nu & 12 \\ n_{\Gamma,1} & 2 \\ n_{\Gamma,2} & 2 \\ n_{\Gamma,3} & 2 \\ n_{\Gamma,4} & 2 \\ n_{\Gamma,5} & 2 \\ n_{\Gamma,6} & 2 \\ n_{M,1} & 6 \\ n_{M,2} & 6 \\ n_{A,1} & 1 \\ n_{A,2} & 2 \\ n_{A,3} & 2 \\ n_{A,4} & 1 \\ n_{A,5} & 2 \\ n_{A,6} & 2 \\ n_{L,1} & 3 \\ n_{L,2} & 3 \\ n_{K,1} & 4 \\ n_{K,2} & 4 \\ n_{K,3} & 4 \\ n_{H,1} & 4 \\ n_{H,2} & 2 \\ n_{H,3} & 4 \end{array} \right) \quad (170)$$

$$\left( \begin{array}{cc} \text{SG170} & a_1 \\ \nu & 12 \\ n_{\Gamma,1} & 2 \\ n_{\Gamma,2} & 2 \\ n_{\Gamma,3} & 2 \\ n_{\Gamma,4} & 2 \\ n_{\Gamma,5} & 2 \\ n_{\Gamma,6} & 2 \\ n_{M,1} & 6 \\ n_{M,2} & 6 \\ n_{A,1} & 1 \\ n_{A,2} & 2 \\ n_{A,3} & 2 \\ n_{A,4} & 1 \\ n_{A,5} & 2 \\ n_{A,6} & 2 \\ n_{L,1} & 3 \\ n_{L,2} & 3 \\ n_{K,1} & 4 \\ n_{K,2} & 4 \\ n_{K,3} & 4 \\ n_{H,1} & 4 \\ n_{H,2} & 2 \\ n_{H,3} & 4 \end{array} \right) \quad (171)$$

$$\left( \begin{array}{cc} \text{SG171} & a_1 \\ \nu & 6 \\ n_{\Gamma,1} & 1 \\ n_{\Gamma,2} & 1 \\ n_{\Gamma,3} & 1 \\ n_{\Gamma,4} & 1 \\ n_{\Gamma,5} & 1 \\ n_{\Gamma,6} & 1 \\ n_{M,1} & 3 \\ n_{M,2} & 3 \\ n_{A,1} & 1 \\ n_{A,2} & 1 \\ n_{A,3} & 1 \\ n_{A,4} & 1 \\ n_{A,5} & 1 \\ n_{A,6} & 1 \\ n_{L,1} & 3 \\ n_{L,2} & 3 \\ n_{K,1} & 2 \\ n_{K,2} & 2 \\ n_{K,3} & 2 \\ n_{H,1} & 2 \\ n_{H,2} & 2 \\ n_{H,3} & 2 \end{array} \right) \quad (172)$$

$$\left( \begin{array}{cc} \text{SG172} & a_1 \\ \nu & 6 \\ n_{\Gamma,1} & 1 \\ n_{\Gamma,2} & 1 \\ n_{\Gamma,3} & 1 \\ n_{\Gamma,4} & 1 \\ n_{\Gamma,5} & 1 \\ n_{\Gamma,6} & 1 \\ n_{M,1} & 3 \\ n_{M,2} & 3 \\ n_{A,1} & 1 \\ n_{A,2} & 1 \\ n_{A,3} & 1 \\ n_{A,4} & 1 \\ n_{A,5} & 1 \\ n_{A,6} & 1 \\ n_{L,1} & 3 \\ n_{L,2} & 3 \\ n_{K,1} & 2 \\ n_{K,2} & 2 \\ n_{K,3} & 2 \\ n_{H,1} & 2 \\ n_{H,2} & 2 \\ n_{H,3} & 2 \end{array} \right) \quad (173)$$

$$\left( \begin{array}{cccc} \text{SG173} & a_1 & a_2 & a_3 \\ \nu & 12 & 4 & 4 \\ n_{\Gamma,1} & 2 & 1 & 1 \\ n_{\Gamma,2} & 2 & 0 & 0 \\ n_{\Gamma,3} & 2 & 1 & 1 \\ n_{\Gamma,4} & 2 & 1 & 1 \\ n_{\Gamma,5} & 2 & 0 & 0 \\ n_{\Gamma,6} & 2 & 1 & 1 \\ n_{M,1} & 6 & 2 & 2 \\ n_{M,2} & 6 & 2 & 2 \\ n_{A,1} & 1 & 0 & 0 \\ n_{A,2} & 2 & 1 & 1 \\ n_{A,3} & 2 & 1 & 1 \\ n_{A,4} & 1 & 0 & 0 \\ n_{A,5} & 2 & 1 & 1 \\ n_{A,6} & 2 & 1 & 1 \\ n_{L,1} & 3 & 1 & 1 \\ n_{L,2} & 3 & 1 & 1 \\ n_{K,1} & 4 & 1 & 2 \\ n_{K,2} & 4 & 2 & 0 \\ n_{K,3} & 4 & 1 & 2 \\ n_{H,1} & 4 & 1 & 2 \\ n_{H,2} & 2 & 1 & 0 \\ n_{H,3} & 4 & 1 & 2 \end{array} \right) \quad (174)$$

$$\left( \begin{array}{cccccccccc} \text{SG174} & a_1 & a_2 & a_3 & a_4 & a_5 & a_6 & a_7 & a_8 & a_9 & a_{10} \\ \nu & 6 & 4 & 4 & 4 & 2 & 2 & 2 & 2 & -30 & -30 \\ n_{\Gamma,1} & 1 & 1 & 1 & 1 & 1 & 1 & 1 & 1 & -9 & -9 \\ n_{\Gamma,2} & 1 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ n_{\Gamma,3} & 1 & 1 & 1 & 1 & 0 & 0 & 0 & 0 & -6 & -6 \\ n_{\Gamma,4} & 1 & 1 & 1 & 1 & 0 & 0 & 0 & 0 & -6 & -6 \\ n_{\Gamma,5} & 1 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ n_{\Gamma,6} & 1 & 1 & 1 & 1 & 1 & 1 & 1 & 1 & -9 & -9 \\ n_{M,1} & 3 & 2 & 2 & 2 & 1 & 1 & 1 & 1 & -15 & -15 \\ n_{M,2} & 3 & 2 & 2 & 2 & 1 & 1 & 1 & 1 & -15 & -15 \\ n_{A,1} & 1 & 1 & 1 & 1 & 0 & 1 & 0 & 1 & -6 & -9 \\ n_{A,2} & 1 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ n_{A,3} & 1 & 1 & 1 & 1 & 1 & 0 & 1 & 0 & -9 & -6 \\ n_{A,4} & 1 & 1 & 1 & 1 & 1 & 0 & 1 & 0 & -9 & -6 \\ n_{A,5} & 1 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ n_{A,6} & 1 & 1 & 1 & 1 & 0 & 1 & 0 & 1 & -6 & -9 \\ n_{L,1} & 3 & 2 & 2 & 2 & 1 & 1 & 1 & 1 & -15 & -15 \\ n_{L,2} & 3 & 2 & 2 & 2 & 1 & 1 & 1 & 1 & -15 & -15 \\ n_{K,1} & 1 & 1 & 0 & 1 & 0 & 0 & 0 & 0 & -3 & -3 \\ n_{K,2} & 1 & 1 & 1 & 0 & 0 & 0 & 1 & 1 & -6 & -6 \\ n_{K,3} & 1 & 0 & 1 & 1 & 0 & 0 & 1 & 1 & -6 & -6 \\ n_{K,4} & 1 & 1 & 0 & 1 & 1 & 1 & 0 & 0 & -6 & -6 \\ n_{K,5} & 1 & 1 & 1 & 0 & 1 & 1 & 0 & 0 & -6 & -6 \\ n_{K,6} & 1 & 0 & 1 & 1 & 0 & 0 & 0 & 0 & -3 & -3 \\ n_{H,1} & 1 & 1 & 0 & 1 & 1 & 0 & 0 & 0 & -6 & -3 \\ n_{H,2} & 1 & 1 & 1 & 0 & 1 & 0 & 0 & 1 & -6 & -6 \\ n_{H,3} & 1 & 0 & 1 & 1 & 0 & 0 & 0 & 1 & -3 & -6 \\ n_{H,4} & 1 & 1 & 0 & 1 & 0 & 1 & 0 & 0 & -3 & -6 \\ n_{H,5} & 1 & 1 & 1 & 0 & 0 & 1 & 1 & 0 & -6 & -6 \\ n_{H,6} & 1 & 0 & 1 & 1 & 0 & 0 & 1 & 0 & -6 & -3 \end{array} \right) \quad (175)$$

SG175	$a_1$	$a_2$	$a_3$	$a_4$	$a_5$	$a_6$	$a_7$	$a_8$	$a_9$	$a_{10}$	$a_{11}$	$a_{12}$	$a_{13}$	$a_{14}$
$\nu$	12	8	6	6	4	4	4	4	2	2	-236	2	228	-144
$n_{\Gamma,1}$	1	1	1	1	1	0	1	1	1	0	-47	1	42	-36
$n_{\Gamma,2}$	1	0	1	1	0	1	0	0	0	1	-23	0	24	-12
$n_{\Gamma,3}$	1	1	1	1	0	0	0	0	0	0	-18	0	18	-12
$n_{\Gamma,4}$	1	1	1	1	0	0	0	0	0	0	-18	0	18	-12
$n_{\Gamma,5}$	1	0	1	1	0	1	0	0	0	1	-23	0	24	-12
$n_{\Gamma,6}$	1	1	1	1	1	0	1	1	1	0	-47	1	42	-36
$n_{\Gamma,7}$	1	1	0	0	1	0	0	0	0	0	-6	0	6	0
$n_{\Gamma,8}$	1	0	0	0	0	1	0	0	0	0	-6	0	6	0
$n_{\Gamma,9}$	1	1	0	0	0	0	1	1	0	0	-18	0	18	-12
$n_{\Gamma,10}$	1	1	0	0	0	0	1	1	0	0	-18	0	18	-12
$n_{\Gamma,11}$	1	0	0	0	0	1	0	0	0	0	-6	0	6	0
$n_{\Gamma,12}$	1	1	0	0	1	0	0	0	0	0	-6	0	6	0
$n_{M,1}$	3	2	1	1	1	1	1	1	1	1	-58	1	54	-36
$n_{M,2}$	3	2	1	1	1	1	1	1	1	1	-58	1	54	-36
$n_{M,3}$	3	2	2	2	1	1	1	1	0	0	-60	0	60	-36
$n_{M,4}$	3	2	2	2	1	1	1	1	0	0	-60	0	60	-36
$n_{A,1}$	1	1	0	1	1	0	0	1	0	0	-29	1	24	-24
$n_{A,2}$	1	0	0	1	0	1	0	0	0	0	-17	0	18	-12
$n_{A,3}$	1	1	0	1	0	0	1	0	0	0	-18	0	18	-12
$n_{A,4}$	1	1	0	1	0	0	1	0	0	0	-18	0	18	-12
$n_{A,5}$	1	0	0	1	0	1	0	0	0	0	-17	0	18	-12
$n_{A,6}$	1	1	0	1	1	0	0	1	0	0	-29	1	24	-24
$n_{A,7}$	1	1	1	0	1	0	1	0	1	0	-24	0	24	-12
$n_{A,8}$	1	0	1	0	0	1	0	0	0	1	-12	0	12	0
$n_{A,9}$	1	1	1	0	0	0	0	1	0	0	-18	0	18	-12
$n_{A,10}$	1	1	1	0	0	0	0	1	0	0	-18	0	18	-12
$n_{A,11}$	1	0	1	0	0	1	0	0	0	1	-12	0	12	0
$n_{A,12}$	1	1	1	0	1	0	1	0	1	0	-24	0	24	-12
$n_{L,1}$	3	2	2	1	1	1	1	1	0	0	-58	1	54	-36
$n_{L,2}$	3	2	2	1	1	1	1	1	0	0	-58	1	54	-36
$n_{L,3}$	3	2	1	2	1	1	1	1	1	1	-60	0	60	-36
$n_{L,4}$	3	2	1	2	1	1	1	1	1	1	-60	0	60	-36
$n_{K,1}$	2	1	1	1	1	0	0	0	1	0	-35	1	30	-24
$n_{K,2}$	2	2	1	1	0	2	1	1	0	1	-47	0	48	-24
$n_{K,3}$	2	1	1	1	1	0	1	1	0	0	-36	0	36	-24
$n_{K,4}$	2	1	1	1	1	0	1	1	0	0	-36	0	36	-24
$n_{K,5}$	2	2	1	1	0	2	1	1	0	1	-47	0	48	-24
$n_{K,6}$	2	1	1	1	1	0	0	0	1	0	-35	1	30	-24
$n_{H,1}$	2	1	1	1	1	0	1	0	0	0	-35	1	30	-24
$n_{H,2}$	2	2	1	1	0	2	1	1	0	1	-47	0	48	-24
$n_{H,3}$	2	1	1	1	1	0	0	1	1	0	-36	0	36	-24
$n_{H,4}$	2	1	1	1	1	0	0	1	1	0	-36	0	36	-24
$n_{H,5}$	2	2	1	1	0	2	1	1	0	1	-47	0	48	-24
$n_{H,6}$	2	1	1	1	1	0	1	0	0	0	-35	1	30	-24

$$\left( \begin{array}{ccccccccc} \text{SG176} & a_1 & a_2 & a_3 & a_4 & a_5 & a_6 & a_7 & a_8 & a_9 \\ \nu & 12 & 12 & 8 & 8 & 4 & 4 & 4 & -52 & 432 \\ n_{\Gamma,1} & 1 & 2 & 1 & 1 & 1 & 1 & 1 & -10 & 84 \\ n_{\Gamma,2} & 1 & 2 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ n_{\Gamma,3} & 1 & 2 & 1 & 1 & 0 & 0 & 1 & -7 & 60 \\ n_{\Gamma,4} & 1 & 2 & 1 & 1 & 0 & 0 & 1 & -7 & 60 \\ n_{\Gamma,5} & 1 & 2 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ n_{\Gamma,6} & 1 & 2 & 1 & 1 & 1 & 1 & 1 & -10 & 84 \\ n_{\Gamma,7} & 1 & 0 & 1 & 1 & 0 & 0 & 0 & -3 & 24 \\ n_{\Gamma,8} & 1 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ n_{\Gamma,9} & 1 & 0 & 1 & 1 & 1 & 1 & 0 & -6 & 48 \\ n_{\Gamma,10} & 1 & 0 & 1 & 1 & 1 & 1 & 0 & -6 & 48 \\ n_{\Gamma,11} & 1 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ n_{\Gamma,12} & 1 & 0 & 1 & 1 & 0 & 0 & 0 & -3 & 24 \\ n_M,1 & 3 & 2 & 2 & 2 & 1 & 1 & 2 & -13 & 108 \\ n_M,2 & 3 & 2 & 2 & 2 & 1 & 1 & 2 & -13 & 108 \\ n_M,3 & 3 & 4 & 2 & 2 & 1 & 1 & 0 & -13 & 108 \\ n_M,4 & 3 & 4 & 2 & 2 & 1 & 1 & 0 & -13 & 108 \\ n_A,1 & 2 & 2 & 2 & 2 & 1 & 1 & 1 & -13 & 108 \\ n_A,2 & 1 & 1 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ n_A,3 & 2 & 2 & 2 & 2 & 1 & 1 & 1 & -13 & 108 \\ n_L,1 & 3 & 3 & 2 & 2 & 1 & 1 & 1 & -13 & 108 \\ n_K,1 & 2 & 2 & 1 & 2 & 0 & 0 & 1 & -7 & 60 \\ n_K,2 & 2 & 2 & 2 & 0 & 1 & 1 & 0 & -6 & 48 \\ n_K,3 & 2 & 2 & 1 & 2 & 1 & 1 & 1 & -13 & 108 \\ n_K,4 & 2 & 2 & 1 & 2 & 1 & 1 & 1 & -13 & 108 \\ n_K,5 & 2 & 2 & 2 & 0 & 1 & 1 & 0 & -6 & 48 \\ n_K,6 & 2 & 2 & 1 & 2 & 0 & 0 & 1 & -7 & 60 \\ n_H,1 & 2 & 2 & 1 & 2 & 0 & 1 & 1 & -10 & 84 \\ n_H,2 & 1 & 1 & 1 & 0 & 0 & 1 & 0 & -3 & 24 \\ n_H,3 & 2 & 2 & 1 & 2 & 0 & 1 & 1 & -10 & 84 \\ n_H,4 & 2 & 2 & 1 & 2 & 1 & 0 & 1 & -10 & 84 \\ n_H,5 & 1 & 1 & 1 & 0 & 1 & 0 & 0 & -3 & 24 \\ n_H,6 & 2 & 2 & 1 & 2 & 1 & 0 & 1 & -10 & 84 \end{array} \right) \quad (177)$$

$$\left( \begin{array}{ccccc} \text{SG177} & a_1 & a_2 & a_3 & a_4 \\ \nu & 6 & 4 & 2 & 2 \\ n_{\Gamma,1} & 1 & 0 & 0 & 1 \\ n_{\Gamma,2} & 1 & 1 & 1 & 0 \\ n_{\Gamma,3} & 1 & 1 & 0 & 0 \\ n_M,1 & 3 & 2 & 1 & 1 \\ n_A,1 & 1 & 0 & 0 & 1 \\ n_A,2 & 1 & 1 & 1 & 0 \\ n_A,3 & 1 & 1 & 0 & 0 \\ n_L,1 & 3 & 2 & 1 & 1 \\ n_K,1 & 1 & 1 & 0 & 1 \\ n_K,2 & 1 & 1 & 0 & 1 \\ n_K,3 & 2 & 1 & 1 & 0 \\ n_H,1 & 1 & 1 & 0 & 1 \\ n_H,2 & 1 & 1 & 0 & 1 \\ n_H,3 & 2 & 1 & 1 & 0 \end{array} \right) \quad (178)$$

$$\left( \begin{array}{cc} \text{SG178} & a_1 \\ \nu & 12 \\ n_{\Gamma,1} & 2 \\ n_{\Gamma,2} & 2 \\ n_{\Gamma,3} & 2 \\ n_{M,1} & 6 \\ n_{A,1} & 1 \\ n_{A,2} & 1 \\ n_{A,3} & 1 \\ n_{A,4} & 1 \\ n_{A,5} & 1 \\ n_{A,6} & 2 \\ n_{L,1} & 3 \\ n_{L,2} & 3 \\ n_{L,3} & 3 \\ n_{L,4} & 3 \\ n_{K,1} & 2 \\ n_{K,2} & 2 \\ n_{K,3} & 4 \\ n_{H,1} & 2 \\ n_{H,2} & 2 \\ n_{H,3} & 4 \end{array} \right) \quad (179)$$

$$\left( \begin{array}{cc} \text{SG179} & a_1 \\ \nu & 12 \\ n_{\Gamma,1} & 2 \\ n_{\Gamma,2} & 2 \\ n_{\Gamma,3} & 2 \\ n_{M,1} & 6 \\ n_{A,1} & 1 \\ n_{A,2} & 1 \\ n_{A,3} & 1 \\ n_{A,4} & 1 \\ n_{A,5} & 1 \\ n_{A,6} & 2 \\ n_{L,1} & 3 \\ n_{L,2} & 3 \\ n_{L,3} & 3 \\ n_{L,4} & 3 \\ n_{K,1} & 2 \\ n_{K,2} & 2 \\ n_{K,3} & 4 \\ n_{H,1} & 2 \\ n_{H,2} & 2 \\ n_{H,3} & 4 \end{array} \right) \quad (180)$$

$$\begin{pmatrix} \text{SG180} & a_1 \\ \nu & 6 \\ n_{\Gamma,1} & 1 \\ n_{\Gamma,2} & 1 \\ n_{\Gamma,3} & 1 \\ n_{M,1} & 3 \\ n_{A,1} & 1 \\ n_{A,2} & 1 \\ n_{A,3} & 1 \\ n_{L,1} & 3 \\ n_{K,1} & 1 \\ n_{K,2} & 1 \\ n_{K,3} & 2 \\ n_{H,1} & 1 \\ n_{H,2} & 1 \\ n_{H,3} & 2 \end{pmatrix} \quad (181)$$

$$\begin{pmatrix} \text{SG181} & a_1 \\ \nu & 6 \\ n_{\Gamma,1} & 1 \\ n_{\Gamma,2} & 1 \\ n_{\Gamma,3} & 1 \\ n_{M,1} & 3 \\ n_{A,1} & 1 \\ n_{A,2} & 1 \\ n_{A,3} & 1 \\ n_{L,1} & 3 \\ n_{K,1} & 1 \\ n_{K,2} & 1 \\ n_{K,3} & 2 \\ n_{H,1} & 1 \\ n_{H,2} & 1 \\ n_{H,3} & 2 \end{pmatrix} \quad (182)$$

$$\left( \begin{array}{cccc} \text{SG182} & a_1 & a_2 & a_3 \\ \nu & 12 & 4 & 4 \\ n_{\Gamma,1} & 2 & 0 & 0 \\ n_{\Gamma,2} & 2 & 1 & 1 \\ n_{\Gamma,3} & 2 & 1 & 1 \\ n_{M,1} & 6 & 2 & 2 \\ n_{A,1} & 1 & 0 & 0 \\ n_{A,2} & 1 & 0 & 0 \\ n_{A,3} & 1 & 0 & 0 \\ n_{A,4} & 1 & 0 & 0 \\ n_{A,5} & 2 & 1 & 1 \\ n_{A,6} & 2 & 1 & 1 \\ n_{L,1} & 3 & 1 & 1 \\ n_{L,2} & 3 & 1 & 1 \\ n_{L,3} & 3 & 1 & 1 \\ n_{L,4} & 3 & 1 & 1 \\ n_{K,1} & 2 & 1 & 0 \\ n_{K,2} & 2 & 1 & 0 \\ n_{K,3} & 4 & 1 & 2 \\ n_{H,1} & 2 & 1 & 0 \\ n_{H,2} & 2 & 1 & 0 \\ n_{H,3} & 4 & 1 & 2 \end{array} \right) \quad (183)$$

$$\left( \begin{array}{ccccc} \text{SG183} & a_1 & a_2 & a_3 & a_4 \\ \nu & 6 & 2 & 2 & 2 \\ n_{\Gamma,1} & 1 & 1 & 1 & 0 \\ n_{\Gamma,2} & 1 & 0 & 0 & 1 \\ n_{\Gamma,3} & 1 & 0 & 0 & 0 \\ n_{M,1} & 3 & 1 & 1 & 1 \\ n_{A,1} & 1 & 1 & 1 & 0 \\ n_{A,2} & 1 & 0 & 0 & 1 \\ n_{A,3} & 1 & 0 & 0 & 0 \\ n_{L,1} & 3 & 1 & 1 & 1 \\ n_{K,1} & 1 & 0 & 1 & 0 \\ n_{K,2} & 1 & 0 & 1 & 0 \\ n_{K,3} & 2 & 1 & 0 & 1 \\ n_{H,1} & 1 & 0 & 1 & 0 \\ n_{H,2} & 1 & 0 & 1 & 0 \\ n_{H,3} & 2 & 1 & 0 & 1 \end{array} \right) \quad (184)$$

$$\left( \begin{array}{c|cccc} \text{SG184} & a_1 & a_2 & a_3 & a_4 \\ \nu & 12 & 8 & 4 & 4 \\ n_{\Gamma,1} & 2 & 0 & 0 & 2 \\ n_{\Gamma,2} & 2 & 2 & 2 & 0 \\ n_{\Gamma,3} & 2 & 2 & 0 & 0 \\ n_{M,1} & 6 & 4 & 2 & 2 \\ n_{A,1} & 1 & 1 & 1 & 0 \\ n_{A,2} & 1 & 1 & 0 & 0 \\ n_{A,3} & 1 & 0 & 0 & 1 \\ n_{L,1} & 3 & 2 & 1 & 1 \\ n_{K,1} & 2 & 2 & 0 & 2 \\ n_{K,2} & 2 & 2 & 0 & 2 \\ n_{K,3} & 4 & 2 & 2 & 0 \\ n_{H,1} & 2 & 2 & 0 & 2 \\ n_{H,2} & 2 & 2 & 0 & 2 \\ n_{H,3} & 2 & 1 & 1 & 0 \end{array} \right) \quad (185)$$

$$\left( \begin{array}{c|ccc} \text{SG185} & a_1 & a_2 & a_3 \\ \nu & 12 & 8 & -4 \\ n_{\Gamma,1} & 2 & 0 & 0 \\ n_{\Gamma,2} & 2 & 2 & -1 \\ n_{\Gamma,3} & 2 & 2 & -1 \\ n_{M,1} & 6 & 4 & -2 \\ n_{A,1} & 1 & 0 & 0 \\ n_{A,2} & 2 & 2 & -1 \\ n_{A,3} & 2 & 2 & -1 \\ n_{L,1} & 3 & 2 & -1 \\ n_{K,1} & 2 & 2 & 0 \\ n_{K,2} & 2 & 2 & 0 \\ n_{K,3} & 4 & 2 & -2 \\ n_{H,1} & 1 & 1 & 0 \\ n_{H,2} & 1 & 1 & 0 \\ n_{H,3} & 2 & 1 & -1 \end{array} \right) \quad (186)$$

$$\left( \begin{array}{c|ccc} \text{SG186} & a_1 & a_2 & a_3 \\ \nu & 12 & -4 & -4 \\ n_{\Gamma,1} & 2 & 0 & 0 \\ n_{\Gamma,2} & 2 & -1 & -1 \\ n_{\Gamma,3} & 2 & -1 & -1 \\ n_{M,1} & 6 & -2 & -2 \\ n_{A,1} & 1 & 0 & 0 \\ n_{A,2} & 2 & -1 & -1 \\ n_{A,3} & 2 & -1 & -1 \\ n_{L,1} & 3 & -1 & -1 \\ n_{K,1} & 2 & -1 & 0 \\ n_{K,2} & 2 & -1 & 0 \\ n_{K,3} & 4 & -1 & -2 \\ n_{H,1} & 2 & -1 & 0 \\ n_{H,2} & 2 & -1 & 0 \\ n_{H,3} & 4 & -1 & -2 \end{array} \right) \quad (187)$$

$$\left( \begin{array}{l} \text{SG187} \quad a_1 \quad a_2 \quad a_3 \quad a_4 \quad a_5 \quad a_6 \quad a_7 \quad a_8 \quad a_9 \quad a_{10} \\ \nu \quad 6 \quad 2 \quad -12 \quad -12 \\ n_{\Gamma,1} \quad 1 \quad 1 \quad 1 \quad 1 \quad 0 \quad 0 \quad 0 \quad 0 \quad -3 \quad -3 \\ n_{\Gamma,2} \quad 1 \quad 0 \quad 0 \quad 0 \quad 1 \quad 1 \quad 1 \quad 1 \quad -3 \quad -3 \\ n_{\Gamma,3} \quad 1 \quad 0 \\ n_{M,1} \quad 3 \quad 1 \quad -6 \quad -6 \\ n_{A,1} \quad 1 \quad 1 \quad 1 \quad 1 \quad 0 \quad 0 \quad 0 \quad 0 \quad -3 \quad -3 \\ n_{A,2} \quad 1 \quad 0 \quad 0 \quad 0 \quad 0 \quad 1 \quad 0 \quad 1 \quad 0 \quad -3 \\ n_{A,3} \quad 1 \quad 0 \quad 0 \quad 0 \quad 1 \quad 0 \quad 1 \quad 0 \quad -3 \quad 0 \\ n_{L,1} \quad 3 \quad 1 \quad -6 \quad -6 \\ n_{K,1} \quad 1 \quad 0 \quad 1 \quad 0 \\ n_{K,2} \quad 1 \quad 0 \quad 0 \quad 1 \quad 0 \quad 0 \quad 1 \quad 1 \quad -3 \quad -3 \\ n_{K,3} \quad 1 \quad 1 \quad 0 \quad 0 \quad 0 \quad 0 \quad 1 \quad 1 \quad -3 \quad -3 \\ n_{K,4} \quad 1 \quad 0 \quad 1 \quad 0 \quad 1 \quad 1 \quad 0 \quad 0 \quad -3 \quad -3 \\ n_{K,5} \quad 1 \quad 0 \quad 0 \quad 1 \quad 1 \quad 1 \quad 0 \quad 0 \quad -3 \quad -3 \\ n_{K,6} \quad 1 \quad 1 \quad 0 \\ n_{H,1} \quad 1 \quad 0 \quad 1 \quad 0 \quad 1 \quad 0 \quad 0 \quad 0 \quad -3 \quad 0 \\ n_{H,2} \quad 1 \quad 0 \quad 0 \quad 1 \quad 1 \quad 0 \quad 0 \quad 1 \quad -3 \quad -3 \\ n_{H,3} \quad 1 \quad 1 \quad 0 \quad 0 \quad 0 \quad 0 \quad 0 \quad 1 \quad 0 \quad -3 \\ n_{H,4} \quad 1 \quad 0 \quad 1 \quad 0 \quad 0 \quad 1 \quad 0 \quad 0 \quad 0 \quad -3 \\ n_{H,5} \quad 1 \quad 0 \quad 0 \quad 1 \quad 0 \quad 1 \quad 1 \quad 0 \quad -3 \quad -3 \\ n_{H,6} \quad 1 \quad 1 \quad 0 \quad 0 \quad 0 \quad 0 \quad 1 \quad 0 \quad -3 \quad 0 \end{array} \right) \quad (188)$$

$$\left( \begin{array}{l} \text{SG188} \quad a_1 \quad a_2 \quad a_3 \quad a_4 \quad a_5 \quad a_6 \quad a_7 \\ \nu \quad 12 \quad 4 \quad 4 \quad 4 \quad 4 \quad 4 \quad -24 \\ n_{\Gamma,1} \quad 2 \quad 0 \quad 0 \quad 0 \quad 0 \quad 0 \quad 0 \\ n_{\Gamma,2} \quad 2 \quad 1 \quad 1 \quad 1 \quad 2 \quad 2 \quad -9 \\ n_{\Gamma,3} \quad 2 \quad 1 \quad 1 \quad 1 \quad 0 \quad 0 \quad -3 \\ n_{M,1} \quad 6 \quad 2 \quad 2 \quad 2 \quad 2 \quad 2 \quad -12 \\ n_{A,1} \quad 1 \quad 0 \quad 0 \quad 0 \quad 0 \quad 0 \quad 0 \\ n_{A,2} \quad 1 \quad 0 \quad 0 \quad 0 \quad 0 \quad 0 \quad 0 \\ n_{A,3} \quad 1 \quad 0 \quad 0 \quad 0 \quad 0 \quad 0 \quad 0 \\ n_{A,4} \quad 1 \quad 0 \quad 0 \quad 0 \quad 0 \quad 0 \quad 0 \\ n_{A,5} \quad 2 \quad 1 \quad 1 \quad 1 \quad 1 \quad 1 \quad -6 \\ n_{A,6} \quad 2 \quad 1 \quad 1 \quad 1 \quad 1 \quad 1 \quad -6 \\ n_{L,1} \quad 3 \quad 1 \quad 1 \quad 1 \quad 1 \quad 1 \quad -6 \\ n_{L,2} \quad 3 \quad 1 \quad 1 \quad 1 \quad 1 \quad 1 \quad -6 \\ n_{L,3} \quad 3 \quad 1 \quad 1 \quad 1 \quad 1 \quad 1 \quad -6 \\ n_{L,4} \quad 3 \quad 1 \quad 1 \quad 1 \quad 1 \quad 1 \quad -6 \\ n_{K,1} \quad 2 \quad 1 \quad 0 \quad 1 \quad 0 \quad 0 \quad 0 \\ n_{K,2} \quad 2 \quad 1 \quad 1 \quad 0 \quad 0 \quad 2 \quad -6 \\ n_{K,3} \quad 2 \quad 0 \quad 1 \quad 1 \quad 0 \quad 2 \quad -6 \\ n_{K,4} \quad 2 \quad 1 \quad 0 \quad 1 \quad 2 \quad 0 \quad -6 \\ n_{K,5} \quad 2 \quad 1 \quad 1 \quad 0 \quad 2 \quad 0 \quad -6 \\ n_{K,6} \quad 2 \quad 0 \quad 1 \quad 1 \quad 0 \quad 0 \quad 0 \\ n_{H,1} \quad 2 \quad 1 \quad 0 \quad 1 \quad 1 \quad 0 \quad -3 \\ n_{H,2} \quad 2 \quad 1 \quad 1 \quad 0 \quad 1 \quad 1 \quad -6 \\ n_{H,3} \quad 2 \quad 0 \quad 1 \quad 1 \quad 0 \quad 1 \quad -3 \\ n_{H,4} \quad 2 \quad 1 \quad 0 \quad 1 \quad 1 \quad 0 \quad -3 \\ n_{H,5} \quad 2 \quad 1 \quad 1 \quad 0 \quad 1 \quad 1 \quad -6 \\ n_{H,6} \quad 2 \quad 0 \quad 1 \quad 1 \quad 0 \quad 1 \quad -3 \end{array} \right) \quad (189)$$

$$\left( \begin{array}{ccccccc} \text{SG189} & a_1 & a_2 & a_3 & a_4 & a_5 & a_6 & a_7 \\ \nu & 6 & 8 & 2 & 4 & 4 & -36 & -36 \\ n_{\Gamma,1} & 1 & 0 & 1 & 0 & 0 & -3 & -3 \\ n_{\Gamma,2} & 1 & 2 & 0 & 2 & 2 & -9 & -9 \\ n_{\Gamma,3} & 1 & 2 & 0 & 0 & 0 & -6 & -6 \\ n_{M,1} & 3 & 4 & 1 & 2 & 2 & -18 & -18 \\ n_{A,1} & 1 & 0 & 1 & 0 & 0 & -3 & -3 \\ n_{A,2} & 1 & 2 & 0 & 0 & 2 & -6 & -9 \\ n_{A,3} & 1 & 2 & 0 & 2 & 0 & -9 & -6 \\ n_{L,1} & 3 & 4 & 1 & 2 & 2 & -18 & -18 \\ n_{K,1} & 1 & 2 & 1 & 1 & 1 & -9 & -9 \\ n_{K,2} & 1 & 1 & 0 & 0 & 0 & -3 & -3 \\ n_{K,3} & 1 & 1 & 0 & 1 & 1 & -6 & -6 \\ n_{H,1} & 1 & 2 & 1 & 1 & 1 & -9 & -9 \\ n_{H,2} & 1 & 1 & 0 & 1 & 0 & -6 & -3 \\ n_{H,3} & 1 & 1 & 0 & 0 & 1 & -3 & -6 \end{array} \right) \quad (190)$$

$$\left( \begin{array}{ccccccc} \text{SG190} & a_1 & a_2 & a_3 & a_4 & a_5 & a_6 \\ \nu & 12 & 8 & 4 & 4 & 4 & -24 \\ n_{\Gamma,1} & 2 & 0 & 0 & 0 & 0 & 0 \\ n_{\Gamma,2} & 2 & 2 & 1 & 2 & 2 & -9 \\ n_{\Gamma,3} & 2 & 2 & 1 & 0 & 0 & -3 \\ n_{M,1} & 6 & 4 & 2 & 2 & 2 & -12 \\ n_{A,1} & 1 & 0 & 0 & 0 & 0 & 0 \\ n_{A,2} & 1 & 0 & 0 & 0 & 0 & 0 \\ n_{A,3} & 1 & 0 & 0 & 0 & 0 & 0 \\ n_{A,4} & 1 & 0 & 0 & 0 & 0 & 0 \\ n_{A,5} & 2 & 2 & 1 & 1 & 1 & -6 \\ n_{A,6} & 2 & 2 & 1 & 1 & 1 & -6 \\ n_{L,1} & 3 & 2 & 1 & 1 & 1 & -6 \\ n_{L,2} & 3 & 2 & 1 & 1 & 1 & -6 \\ n_{L,3} & 3 & 2 & 1 & 1 & 1 & -6 \\ n_{L,4} & 3 & 2 & 1 & 1 & 1 & -6 \\ n_{K,1} & 2 & 2 & 0 & 1 & 1 & -6 \\ n_{K,2} & 2 & 1 & 1 & 0 & 0 & 0 \\ n_{K,3} & 2 & 1 & 1 & 1 & 1 & -6 \\ n_{H,1} & 1 & 1 & 0 & 0 & 1 & -3 \\ n_{H,2} & 1 & 1 & 0 & 0 & 1 & -3 \\ n_{H,3} & 1 & 1 & 0 & 1 & 0 & -3 \\ n_{H,4} & 1 & 1 & 0 & 1 & 0 & -3 \\ n_{H,5} & 2 & 1 & 1 & 1 & 0 & -3 \\ n_{H,6} & 2 & 1 & 1 & 0 & 1 & -3 \end{array} \right) \quad (191)$$

$$\left( \begin{array}{c|cccccccccccccc} \text{SG191} & a_1 & a_2 & a_3 & a_4 & a_5 & a_6 & a_7 & a_8 & a_9 & a_{10} & a_{11} & a_{12} & a_{13} & a_{14} \\ \nu & 12 & 4 & 6 & 6 & 4 & 4 & 4 & 4 & 2 & 2 & -260 & 2 & 252 & -144 \\ n_{\Gamma,1} & 1 & 1 & 1 & 1 & 1 & 0 & 0 & 0 & 1 & 0 & -29 & 1 & 24 & -12 \\ n_{\Gamma,2} & 1 & 0 & 1 & 1 & 0 & 1 & 1 & 1 & 0 & 1 & -47 & 0 & 48 & -36 \\ n_{\Gamma,3} & 1 & 0 & 1 & 1 & 0 & 0 & 0 & 0 & 0 & 0 & -18 & 0 & 18 & -12 \\ n_{\Gamma,4} & 1 & 1 & 0 & 0 & 1 & 0 & 0 & 0 & 0 & 0 & -12 & 0 & 12 & 0 \\ n_{\Gamma,5} & 1 & 0 & 0 & 0 & 0 & 1 & 0 & 0 & 0 & 0 & -6 & 0 & 6 & 0 \\ n_{\Gamma,6} & 1 & 0 & 0 & 0 & 0 & 0 & 1 & 1 & 0 & 0 & -18 & 0 & 18 & -12 \\ n_{M,1} & 3 & 1 & 1 & 1 & 1 & 1 & 1 & 1 & 1 & 1 & -64 & 1 & 60 & -36 \\ n_{M,2} & 3 & 1 & 2 & 2 & 1 & 1 & 1 & 1 & 0 & 0 & -66 & 0 & 66 & -36 \\ n_{A,1} & 1 & 1 & 0 & 1 & 1 & 0 & 0 & 0 & 0 & 0 & -23 & 1 & 18 & -12 \\ n_{A,2} & 1 & 0 & 0 & 1 & 0 & 1 & 0 & 1 & 0 & 0 & -29 & 0 & 30 & -24 \\ n_{A,3} & 1 & 0 & 0 & 1 & 0 & 0 & 1 & 0 & 0 & 0 & -18 & 0 & 18 & -12 \\ n_{A,4} & 1 & 1 & 1 & 0 & 1 & 0 & 0 & 0 & 1 & 0 & -18 & 0 & 18 & 0 \\ n_{A,5} & 1 & 0 & 1 & 0 & 0 & 1 & 1 & 0 & 0 & 1 & -24 & 0 & 24 & -12 \\ n_{A,6} & 1 & 0 & 1 & 0 & 0 & 0 & 0 & 1 & 0 & 0 & -18 & 0 & 18 & -12 \\ n_{L,1} & 3 & 1 & 2 & 1 & 1 & 1 & 1 & 1 & 0 & 0 & -64 & 1 & 60 & -36 \\ n_{L,2} & 3 & 1 & 1 & 2 & 1 & 1 & 1 & 1 & 1 & 1 & -66 & 0 & 66 & -36 \\ n_{K,1} & 2 & 0 & 1 & 1 & 2 & 0 & 1 & 1 & 1 & 0 & -47 & 1 & 42 & -24 \\ n_{K,2} & 2 & 1 & 1 & 1 & 0 & 1 & 0 & 0 & 0 & 1 & -41 & 0 & 42 & -24 \\ n_{K,3} & 2 & 1 & 1 & 1 & 0 & 1 & 1 & 1 & 0 & 0 & -42 & 0 & 42 & -24 \\ n_{H,1} & 2 & 0 & 1 & 1 & 2 & 0 & 1 & 1 & 1 & 0 & -47 & 1 & 42 & -24 \\ n_{H,2} & 2 & 1 & 1 & 1 & 0 & 1 & 1 & 0 & 0 & 0 & -41 & 0 & 42 & -24 \\ n_{H,3} & 2 & 1 & 1 & 1 & 0 & 1 & 0 & 1 & 0 & 1 & -42 & 0 & 42 & -24 \end{array} \right) \quad (192)$$

$$\left( \begin{array}{c|cccccccccc} \text{SG192} & a_1 & a_2 & a_3 & a_4 & a_5 & a_6 & a_7 & a_8 & a_9 \\ \nu & 12 & 8 & 12 & 4 & 4 & 8 & 4 & 4 & -336 \\ n_{\Gamma,1} & 1 & 0 & 2 & 0 & 1 & 0 & 0 & 2 & -36 \\ n_{\Gamma,2} & 1 & 1 & 2 & 1 & 0 & 2 & 2 & 0 & -60 \\ n_{\Gamma,3} & 1 & 1 & 2 & 0 & 0 & 0 & 0 & 0 & -24 \\ n_{\Gamma,4} & 1 & 0 & 0 & 0 & 1 & 0 & 0 & 0 & -12 \\ n_{\Gamma,5} & 1 & 1 & 0 & 1 & 0 & 0 & 0 & 0 & -12 \\ n_{\Gamma,6} & 1 & 1 & 0 & 0 & 0 & 2 & 0 & 0 & -24 \\ n_{M,1} & 3 & 2 & 2 & 1 & 1 & 2 & 2 & 2 & -84 \\ n_{M,2} & 3 & 2 & 4 & 1 & 1 & 2 & 0 & 0 & -84 \\ n_{A,1} & 1 & 0 & 1 & 0 & 1 & 0 & 0 & 1 & -24 \\ n_{A,2} & 1 & 0 & 1 & 0 & 1 & 0 & 0 & 1 & -24 \\ n_{A,3} & 1 & 1 & 1 & 0 & 0 & 1 & 0 & 0 & -24 \\ n_{A,4} & 1 & 1 & 1 & 1 & 0 & 1 & 1 & 0 & -36 \\ n_{A,5} & 1 & 1 & 1 & 0 & 0 & 1 & 0 & 0 & -24 \\ n_{A,6} & 1 & 1 & 1 & 1 & 0 & 1 & 1 & 0 & -36 \\ n_{L,1} & 3 & 2 & 3 & 1 & 1 & 2 & 1 & 1 & -84 \\ n_{L,2} & 3 & 2 & 3 & 1 & 1 & 2 & 1 & 1 & -84 \\ n_{K,1} & 2 & 2 & 2 & 0 & 2 & 2 & 0 & 2 & -72 \\ n_{K,2} & 2 & 1 & 2 & 1 & 0 & 0 & 2 & 0 & -48 \\ n_{K,3} & 2 & 1 & 2 & 1 & 0 & 2 & 0 & 0 & -48 \\ n_{H,1} & 1 & 1 & 1 & 0 & 1 & 1 & 0 & 1 & -36 \\ n_{H,2} & 1 & 1 & 1 & 0 & 1 & 1 & 0 & 1 & -36 \\ n_{H,3} & 1 & 1 & 1 & 0 & 1 & 1 & 0 & 1 & -36 \\ n_{H,4} & 1 & 1 & 1 & 0 & 1 & 1 & 0 & 1 & -36 \\ n_{H,5} & 2 & 1 & 2 & 1 & 0 & 1 & 1 & 0 & -48 \\ n_{H,6} & 2 & 1 & 2 & 1 & 0 & 1 & 1 & 0 & -48 \end{array} \right) \quad (193)$$

$$\left( \begin{array}{cccccccccc} \text{SG193} & a_1 & a_2 & a_3 & a_4 & a_5 & a_6 & a_7 & a_8 \\ \nu & 12 & 8 & 12 & 4 & 8 & 4 & -32 & 240 \\ n_{\Gamma,1} & 1 & 0 & 2 & 1 & 0 & 0 & -3 & 24 \\ n_{\Gamma,2} & 1 & 1 & 2 & 0 & 2 & 1 & -2 & 12 \\ n_{\Gamma,3} & 1 & 1 & 2 & 0 & 0 & 1 & 1 & -12 \\ n_{\Gamma,4} & 1 & 0 & 0 & 1 & 0 & 0 & -3 & 24 \\ n_{\Gamma,5} & 1 & 1 & 0 & 0 & 0 & 0 & -3 & 24 \\ n_{\Gamma,6} & 1 & 1 & 0 & 0 & 2 & 0 & -6 & 48 \\ n_{M,1} & 3 & 2 & 2 & 1 & 2 & 2 & -8 & 60 \\ n_{M,2} & 3 & 2 & 4 & 1 & 2 & 0 & -8 & 60 \\ n_{A,1} & 1 & 0 & 1 & 1 & 0 & 0 & -3 & 24 \\ n_{A,2} & 1 & 0 & 1 & 1 & 0 & 0 & -3 & 24 \\ n_{A,3} & 2 & 2 & 2 & 0 & 2 & 1 & -5 & 36 \\ n_{L,1} & 3 & 2 & 3 & 1 & 2 & 1 & -8 & 60 \\ n_{L,2} & 3 & 2 & 3 & 1 & 2 & 1 & -8 & 60 \\ n_{K,1} & 2 & 2 & 2 & 2 & 2 & 0 & -12 & 96 \\ n_{K,2} & 2 & 1 & 2 & 0 & 0 & 1 & 1 & -12 \\ n_{K,3} & 2 & 1 & 2 & 0 & 2 & 1 & -5 & 36 \\ n_{H,1} & 1 & 1 & 1 & 1 & 1 & 0 & -6 & 48 \\ n_{H,2} & 2 & 1 & 2 & 0 & 1 & 1 & -2 & 12 \\ n_{H,3} & 2 & 1 & 2 & 0 & 1 & 1 & -2 & 12 \end{array} \right) \quad (194)$$

$$\left( \begin{array}{cccccccccc} \text{SG194} & a_1 & a_2 & a_3 & a_4 & a_5 & a_6 & a_7 & a_8 & a_9 \\ \nu & 12 & 12 & 4 & 4 & 4 & 4 & -4 & 4 & 0 \\ n_{\Gamma,1} & 1 & 2 & 1 & 1 & 0 & 0 & -3 & 0 & 12 \\ n_{\Gamma,2} & 1 & 2 & 0 & 0 & 1 & 1 & 2 & 1 & -12 \\ n_{\Gamma,3} & 1 & 2 & 0 & 0 & 0 & 0 & 5 & 1 & -24 \\ n_{\Gamma,4} & 1 & 0 & 1 & 1 & 0 & 0 & -3 & 0 & 12 \\ n_{\Gamma,5} & 1 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ n_{\Gamma,6} & 1 & 0 & 0 & 0 & 1 & 1 & -3 & 0 & 12 \\ n_{M,1} & 3 & 2 & 1 & 1 & 1 & 1 & 0 & 2 & -12 \\ n_{M,2} & 3 & 4 & 1 & 1 & 1 & 1 & -2 & 0 & 12 \\ n_{A,1} & 1 & 1 & 1 & 1 & 0 & 0 & -3 & 0 & 12 \\ n_{A,2} & 1 & 1 & 1 & 1 & 0 & 0 & -3 & 0 & 12 \\ n_{A,3} & 2 & 2 & 0 & 0 & 1 & 1 & 2 & 1 & -12 \\ n_{L,1} & 3 & 3 & 1 & 1 & 1 & 1 & -1 & 1 & 0 \\ n_{L,2} & 3 & 3 & 1 & 1 & 1 & 1 & -1 & 1 & 0 \\ n_{K,1} & 2 & 2 & 0 & 2 & 1 & 1 & -6 & 0 & 24 \\ n_{K,2} & 2 & 2 & 1 & 0 & 0 & 0 & 5 & 1 & -24 \\ n_{K,3} & 2 & 2 & 1 & 0 & 1 & 1 & -1 & 1 & 0 \\ n_{H,1} & 1 & 1 & 0 & 1 & 0 & 1 & -3 & 0 & 12 \\ n_{H,2} & 1 & 1 & 0 & 1 & 0 & 1 & -3 & 0 & 12 \\ n_{H,3} & 1 & 1 & 0 & 1 & 1 & 0 & -3 & 0 & 12 \\ n_{H,4} & 1 & 1 & 0 & 1 & 1 & 0 & -3 & 0 & 12 \\ n_{H,5} & 2 & 2 & 1 & 0 & 1 & 0 & 2 & 1 & -12 \\ n_{H,6} & 2 & 2 & 1 & 0 & 0 & 1 & 2 & 1 & -12 \end{array} \right) \quad (195)$$

$$\left( \begin{array}{ccc} \text{SG195} & a_1 & a_2 \\ \nu & 6 & 8 \\ n_{\Gamma,1} & 1 & 2 \\ n_{\Gamma,2} & 1 & 1 \\ n_{\Gamma,3} & 1 & 1 \\ n_{X,1} & 3 & 4 \\ n_{M,1} & 3 & 4 \\ n_{R,1} & 1 & 2 \\ n_{R,2} & 1 & 1 \\ n_{R,3} & 1 & 1 \end{array} \right) \quad (196)$$

$$\left( \begin{array}{ccc} \text{SG196} & a_1 & a_2 \\ \nu & 6 & 8 \\ n_{\Gamma,1} & 1 & 2 \\ n_{\Gamma,2} & 1 & 1 \\ n_{\Gamma,3} & 1 & 1 \\ n_{X,1} & 3 & 4 \\ n_{L,1} & 2 & 3 \\ n_{L,2} & 1 & 1 \\ n_{L,3} & 2 & 3 \\ n_{W,1} & 3 & 4 \\ n_{W,2} & 3 & 4 \end{array} \right) \quad (197)$$

$$\left( \begin{array}{ccc} \text{SG197} & a_1 & a_2 \\ \nu & 6 & 8 \\ n_{\Gamma,1} & 1 & 2 \\ n_{\Gamma,2} & 1 & 1 \\ n_{\Gamma,3} & 1 & 1 \\ n_{H,1} & 1 & 2 \\ n_{H,2} & 1 & 1 \\ n_{H,3} & 1 & 1 \\ n_{P,1} & 1 & 2 \\ n_{P,2} & 1 & 1 \\ n_{P,3} & 1 & 1 \\ n_{N,1} & 3 & 4 \\ n_{N,2} & 3 & 4 \end{array} \right) \quad (198)$$

$$\left( \begin{array}{ccc} \text{SG198} & a_1 & a_2 \\ \nu & 24 & 8 \\ n_{\Gamma,1} & 4 & 2 \\ n_{\Gamma,2} & 4 & 1 \\ n_{\Gamma,3} & 4 & 1 \\ n_{X,1} & 6 & 2 \\ n_{X,2} & 6 & 2 \\ n_{X,3} & 6 & 2 \\ n_{X,4} & 6 & 2 \\ n_{M,1} & 6 & 2 \\ n_{R,1} & 1 & 0 \\ n_{R,2} & 2 & 1 \\ n_{R,3} & 2 & 1 \\ n_{R,4} & 3 & 1 \end{array} \right) \quad (199)$$

$$\left( \begin{array}{l} \text{SG199} \quad a_1 \quad a_2 \\ \nu \quad 12 \quad 8 \\ n_{\Gamma,1} \quad 2 \quad 2 \\ n_{\Gamma,2} \quad 2 \quad 1 \\ n_{\Gamma,3} \quad 2 \quad 1 \\ n_{H,1} \quad 2 \quad 2 \\ n_{H,2} \quad 2 \quad 1 \\ n_{H,3} \quad 2 \quad 1 \\ n_{P,1} \quad 1 \quad 0 \\ n_{P,2} \quad 1 \quad 1 \\ n_{P,3} \quad 1 \quad 1 \\ n_{P,4} \quad 3 \quad 2 \\ n_{N,1} \quad 6 \quad 4 \\ n_{N,2} \quad 6 \quad 4 \end{array} \right) \quad (200)$$

$$\left( \begin{array}{l} \text{SG200} \quad a_1 \quad a_2 \quad a_3 \quad a_4 \quad a_5 \quad a_6 \quad a_7 \quad a_8 \\ \nu \quad 12 \quad 16 \quad 6 \quad 6 \quad 2 \quad -10 \quad 12 \quad -8 \\ n_{\Gamma,1} \quad 1 \quad 2 \quad 1 \quad 1 \quad 1 \quad -5 \quad 6 \quad -4 \\ n_{\Gamma,2} \quad 1 \quad 1 \quad 1 \quad 1 \quad 0 \quad 0 \quad 0 \quad 0 \\ n_{\Gamma,3} \quad 1 \quad 1 \quad 1 \quad 1 \quad 0 \quad 0 \quad 0 \quad 0 \\ n_{\Gamma,4} \quad 1 \quad 2 \quad 0 \quad 0 \quad 0 \quad 0 \quad 0 \quad 0 \\ n_{\Gamma,5} \quad 1 \quad 1 \quad 0 \quad 0 \quad 0 \quad 0 \quad 0 \quad 0 \\ n_{\Gamma,6} \quad 1 \quad 1 \quad 0 \quad 0 \quad 0 \quad 0 \quad 0 \quad 0 \\ n_{X,1} \quad 3 \quad 4 \quad 2 \quad 1 \quad 0 \quad -1 \quad 2 \quad 0 \\ n_{X,2} \quad 3 \quad 4 \quad 1 \quad 2 \quad 1 \quad -4 \quad 4 \quad -4 \\ n_{M,1} \quad 3 \quad 4 \quad 1 \quad 1 \quad 1 \quad -3 \quad 4 \quad -4 \\ n_{M,2} \quad 3 \quad 4 \quad 2 \quad 2 \quad 0 \quad -2 \quad 2 \quad 0 \\ n_{R,1} \quad 1 \quad 2 \quad 0 \quad 1 \quad 0 \quad -3 \quad 4 \quad -4 \\ n_{R,2} \quad 1 \quad 1 \quad 0 \quad 1 \quad 0 \quad 0 \quad 0 \quad 0 \\ n_{R,3} \quad 1 \quad 1 \quad 0 \quad 1 \quad 0 \quad 0 \quad 0 \quad 0 \\ n_{R,4} \quad 1 \quad 2 \quad 1 \quad 0 \quad 1 \quad -2 \quad 2 \quad 0 \\ n_{R,5} \quad 1 \quad 1 \quad 1 \quad 0 \quad 0 \quad 0 \quad 0 \quad 0 \\ n_{R,6} \quad 1 \quad 1 \quad 1 \quad 0 \quad 0 \quad 0 \quad 0 \quad 0 \end{array} \right) \quad (201)$$

$$\left( \begin{array}{l} \text{SG201} \quad a_1 \quad a_2 \quad a_3 \quad a_4 \quad a_5 \quad a_6 \\ \nu \quad 12 \quad 16 \quad 8 \quad -16 \quad 24 \quad -32 \\ n_{\Gamma,1} \quad 1 \quad 2 \quad 2 \quad -6 \quad 8 \quad -8 \\ n_{\Gamma,2} \quad 1 \quad 1 \quad 1 \quad -1 \quad 2 \quad -4 \\ n_{\Gamma,3} \quad 1 \quad 1 \quad 1 \quad -1 \quad 2 \quad -4 \\ n_{\Gamma,4} \quad 1 \quad 2 \quad 0 \quad 0 \quad 0 \quad 0 \\ n_{\Gamma,5} \quad 1 \quad 1 \quad 0 \quad 0 \quad 0 \quad 0 \\ n_{\Gamma,6} \quad 1 \quad 1 \quad 0 \quad 0 \quad 0 \quad 0 \\ n_{X,1} \quad 3 \quad 4 \quad 2 \quad -4 \quad 6 \quad -8 \\ n_{X,2} \quad 3 \quad 4 \quad 2 \quad -4 \quad 6 \quad -8 \\ n_{M,1} \quad 3 \quad 4 \quad 2 \quad -4 \quad 6 \quad -8 \\ n_{M,2} \quad 3 \quad 4 \quad 2 \quad -4 \quad 6 \quad -8 \\ n_{R,1} \quad 1 \quad 2 \quad 0 \quad -2 \quad 4 \quad -4 \\ n_{R,2} \quad 1 \quad 1 \quad 0 \quad 1 \quad 0 \quad 0 \\ n_{R,3} \quad 1 \quad 1 \quad 0 \quad 1 \quad 0 \quad 0 \\ n_{R,4} \quad 1 \quad 2 \quad 2 \quad -4 \quad 4 \quad -4 \\ n_{R,5} \quad 1 \quad 1 \quad 1 \quad -2 \quad 2 \quad -4 \\ n_{R,6} \quad 1 \quad 1 \quad 1 \quad -2 \quad 2 \quad -4 \end{array} \right) \quad (202)$$

$$\left( \begin{array}{l} \text{SG202} \quad a_1 \quad a_2 \quad a_3 \quad a_4 \quad a_5 \quad a_6 \quad a_7 \\ \nu \quad 12 \quad 16 \quad 12 \quad 2 \quad 4 \quad 2 \quad -32 \\ n_{\Gamma,1} \quad 1 \quad 2 \quad 2 \quad 1 \quad 0 \quad 1 \quad -8 \\ n_{\Gamma,2} \quad 1 \quad 1 \quad 2 \quad 0 \quad 1 \quad 0 \quad -4 \\ n_{\Gamma,3} \quad 1 \quad 1 \quad 2 \quad 0 \quad 1 \quad 0 \quad -4 \\ n_{\Gamma,4} \quad 1 \quad 2 \quad 0 \quad 0 \quad 0 \quad 0 \quad 0 \\ n_{\Gamma,5} \quad 1 \quad 1 \quad 0 \quad 0 \quad 0 \quad 0 \quad 0 \\ n_{\Gamma,6} \quad 1 \quad 1 \quad 0 \quad 0 \quad 0 \quad 0 \quad 0 \\ n_{X,1} \quad 3 \quad 4 \quad 2 \quad 1 \quad 2 \quad 1 \quad -12 \\ n_{X,2} \quad 3 \quad 4 \quad 4 \quad 0 \quad 0 \quad 0 \quad -4 \\ n_{L,1} \quad 1 \quad 1 \quad 1 \quad 0 \quad 1 \quad 0 \quad -4 \\ n_{L,2} \quad 2 \quad 3 \quad 2 \quad 0 \quad 0 \quad 1 \quad -4 \\ n_{L,3} \quad 2 \quad 3 \quad 2 \quad 1 \quad 1 \quad 0 \quad -8 \\ n_{L,4} \quad 1 \quad 1 \quad 1 \quad 0 \quad 0 \quad 0 \quad 0 \\ n_{L,5} \quad 2 \quad 3 \quad 2 \quad 1 \quad 1 \quad 0 \quad -8 \\ n_{L,6} \quad 2 \quad 3 \quad 2 \quad 0 \quad 0 \quad 1 \quad -4 \\ n_{W,1} \quad 6 \quad 8 \quad 6 \quad 1 \quad 2 \quad 1 \quad -16 \end{array} \right) \quad (203)$$

$$\left( \begin{array}{l} \text{SG203} \quad a_1 \quad a_2 \quad a_3 \quad a_4 \quad a_5 \quad a_6 \\ \nu \quad 12 \quad 16 \quad 8 \quad 8 \quad 8 \quad -48 \\ n_{\Gamma,1} \quad 1 \quad 2 \quad 2 \quad 0 \quad 2 \quad -8 \\ n_{\Gamma,2} \quad 1 \quad 1 \quad 1 \quad 2 \quad 1 \quad -8 \\ n_{\Gamma,3} \quad 1 \quad 1 \quad 1 \quad 2 \quad 1 \quad -8 \\ n_{\Gamma,4} \quad 1 \quad 2 \quad 0 \quad 0 \quad 0 \quad 0 \\ n_{\Gamma,5} \quad 1 \quad 1 \quad 0 \quad 0 \quad 0 \quad 0 \\ n_{\Gamma,6} \quad 1 \quad 1 \quad 0 \quad 0 \quad 0 \quad 0 \\ n_{X,1} \quad 3 \quad 4 \quad 2 \quad 2 \quad 2 \quad -12 \\ n_{X,2} \quad 3 \quad 4 \quad 2 \quad 2 \quad 2 \quad -12 \\ n_{L,1} \quad 1 \quad 1 \quad 0 \quad 1 \quad 1 \quad -4 \\ n_{L,2} \quad 2 \quad 3 \quad 2 \quad 2 \quad 1 \quad -12 \\ n_{L,3} \quad 2 \quad 3 \quad 1 \quad 0 \quad 2 \quad -4 \\ n_{L,4} \quad 1 \quad 1 \quad 1 \quad 1 \quad 0 \quad -4 \\ n_{L,5} \quad 2 \quad 3 \quad 1 \quad 0 \quad 2 \quad -4 \\ n_{L,6} \quad 2 \quad 3 \quad 2 \quad 2 \quad 1 \quad -12 \\ n_{W,1} \quad 3 \quad 4 \quad 2 \quad 2 \quad 2 \quad -12 \\ n_{W,2} \quad 3 \quad 4 \quad 2 \quad 2 \quad 2 \quad -12 \\ n_{W,3} \quad 3 \quad 4 \quad 2 \quad 2 \quad 2 \quad -12 \\ n_{W,4} \quad 3 \quad 4 \quad 2 \quad 2 \quad 2 \quad -12 \end{array} \right) \quad (204)$$

$$\left( \begin{array}{ccccccc} \text{SG204} & a_1 & a_2 & a_3 & a_4 & a_5 & a_6 & a_7 \\ \nu & 12 & 16 & 8 & -16 & 6 & 12 & -32 \\ n_{\Gamma,1} & 1 & 2 & 2 & -6 & 1 & 6 & -8 \\ n_{\Gamma,2} & 1 & 1 & 1 & -1 & 1 & 0 & -4 \\ n_{\Gamma,3} & 1 & 1 & 1 & -1 & 1 & 0 & -4 \\ n_{\Gamma,4} & 1 & 2 & 0 & 0 & 0 & 0 & 0 \\ n_{\Gamma,5} & 1 & 1 & 0 & 0 & 0 & 0 & 0 \\ n_{\Gamma,6} & 1 & 1 & 0 & 0 & 0 & 0 & 0 \\ n_{H,1} & 1 & 2 & 0 & -2 & 1 & 2 & -4 \\ n_{H,2} & 1 & 1 & 0 & 1 & 1 & -2 & 0 \\ n_{H,3} & 1 & 1 & 0 & 1 & 1 & -2 & 0 \\ n_{H,4} & 1 & 2 & 2 & -4 & 0 & 4 & -4 \\ n_{H,5} & 1 & 1 & 1 & -2 & 0 & 2 & -4 \\ n_{H,6} & 1 & 1 & 1 & -2 & 0 & 2 & -4 \\ n_{P,1} & 2 & 4 & 2 & -6 & 1 & 6 & -8 \\ n_{P,2} & 2 & 2 & 1 & -1 & 1 & 0 & -4 \\ n_{P,3} & 2 & 2 & 1 & -1 & 1 & 0 & -4 \\ n_{N,1} & 3 & 4 & 2 & -4 & 1 & 4 & -8 \\ n_{N,2} & 3 & 4 & 2 & -4 & 1 & 4 & -8 \\ n_{N,3} & 3 & 4 & 2 & -4 & 2 & 2 & -8 \\ n_{N,4} & 3 & 4 & 2 & -4 & 2 & 2 & -8 \end{array} \right) \quad (205)$$

$$\left( \begin{array}{ccccccc} \text{SG205} & a_1 & a_2 & a_3 & a_4 & a_5 & a_6 \\ \nu & 48 & 16 & 8 & 8 & 8 & -96 \\ n_{\Gamma,1} & 4 & 2 & 2 & 0 & 2 & -12 \\ n_{\Gamma,2} & 4 & 1 & 1 & 2 & 1 & -12 \\ n_{\Gamma,3} & 4 & 1 & 1 & 2 & 1 & -12 \\ n_{\Gamma,4} & 4 & 2 & 0 & 0 & 0 & -4 \\ n_{\Gamma,5} & 4 & 1 & 0 & 0 & 0 & -4 \\ n_{\Gamma,6} & 4 & 1 & 0 & 0 & 0 & -4 \\ n_{X,1} & 12 & 4 & 2 & 2 & 2 & -24 \\ n_{X,2} & 12 & 4 & 2 & 2 & 2 & -24 \\ n_{M,1} & 6 & 2 & 1 & 1 & 1 & -12 \\ n_{M,2} & 6 & 2 & 1 & 1 & 1 & -12 \\ n_{R,1} & 1 & 0 & 0 & 0 & 0 & 0 \\ n_{R,2} & 2 & 1 & 0 & 0 & 1 & -4 \\ n_{R,3} & 2 & 1 & 0 & 0 & 1 & -4 \\ n_{R,4} & 3 & 1 & 0 & 0 & 1 & -4 \\ n_{R,5} & 1 & 0 & 0 & 1 & 0 & -4 \\ n_{R,6} & 2 & 1 & 1 & 0 & 0 & -4 \\ n_{R,7} & 2 & 1 & 1 & 0 & 0 & -4 \\ n_{R,8} & 3 & 1 & 1 & 1 & 0 & -8 \end{array} \right) \quad (206)$$

$$\left( \begin{array}{l} \text{SG206} \quad a_1 \quad a_2 \quad a_3 \quad a_4 \quad a_5 \quad a_6 \\ \nu \quad 24 \quad 16 \quad 8 \quad -40 \quad 48 \quad -32 \\ n_{\Gamma,1} \quad 2 \quad 2 \quad 2 \quad -8 \quad 10 \quad -8 \\ n_{\Gamma,2} \quad 2 \quad 1 \quad 1 \quad -3 \quad 4 \quad -4 \\ n_{\Gamma,3} \quad 2 \quad 1 \quad 1 \quad -3 \quad 4 \quad -4 \\ n_{\Gamma,4} \quad 2 \quad 2 \quad 0 \quad -2 \quad 2 \quad 0 \\ n_{\Gamma,5} \quad 2 \quad 1 \quad 0 \quad -2 \quad 2 \quad 0 \\ n_{\Gamma,6} \quad 2 \quad 1 \quad 0 \quad -2 \quad 2 \quad 0 \\ n_{H,1} \quad 2 \quad 2 \quad 0 \quad -4 \quad 6 \quad -4 \\ n_{H,2} \quad 2 \quad 1 \quad 0 \quad -1 \quad 2 \quad 0 \\ n_{H,3} \quad 2 \quad 1 \quad 0 \quad -1 \quad 2 \quad 0 \\ n_{H,4} \quad 2 \quad 2 \quad 2 \quad -6 \quad 6 \quad -4 \\ n_{H,5} \quad 2 \quad 1 \quad 1 \quad -4 \quad 4 \quad -4 \\ n_{H,6} \quad 2 \quad 1 \quad 1 \quad -4 \quad 4 \quad -4 \\ n_{P,1} \quad 1 \quad 0 \quad 0 \quad 0 \quad 0 \quad 0 \\ n_{P,2} \quad 2 \quad 2 \quad 1 \quad -5 \quad 6 \quad -4 \\ n_{P,3} \quad 2 \quad 2 \quad 1 \quad -5 \quad 6 \quad -4 \\ n_{N,1} \quad 6 \quad 4 \quad 2 \quad -10 \quad 12 \quad -8 \end{array} \right) \quad (207)$$

$$\left( \begin{array}{l} \text{SG207} \quad a_1 \quad a_2 \quad a_3 \quad a_4 \\ \nu \quad 12 \quad 8 \quad 6 \quad 6 \\ n_{\Gamma,1} \quad 1 \quad 1 \quad 1 \quad 1 \\ n_{\Gamma,2} \quad 1 \quad 1 \quad 0 \quad 0 \\ n_{\Gamma,3} \quad 2 \quad 1 \quad 1 \quad 1 \\ n_{X,1} \quad 3 \quad 2 \quad 2 \quad 2 \\ n_{X,2} \quad 3 \quad 2 \quad 1 \quad 1 \\ n_{M,1} \quad 3 \quad 2 \quad 1 \quad 2 \\ n_{M,2} \quad 3 \quad 2 \quad 2 \quad 1 \\ n_{R,1} \quad 1 \quad 1 \quad 0 \quad 1 \\ n_{R,2} \quad 1 \quad 1 \quad 1 \quad 0 \\ n_{R,3} \quad 2 \quad 1 \quad 1 \quad 1 \end{array} \right) \quad (208)$$

$$\left( \begin{array}{l} \text{SG208} \quad a_1 \quad a_2 \\ \nu \quad 12 \quad 8 \\ n_{\Gamma,1} \quad 1 \quad 1 \\ n_{\Gamma,2} \quad 1 \quad 1 \\ n_{\Gamma,3} \quad 2 \quad 1 \\ n_{X,1} \quad 3 \quad 2 \\ n_{X,2} \quad 3 \quad 2 \\ n_{M,1} \quad 3 \quad 2 \\ n_{M,2} \quad 3 \quad 2 \\ n_{R,1} \quad 1 \quad 1 \\ n_{R,2} \quad 1 \quad 1 \\ n_{R,3} \quad 2 \quad 1 \end{array} \right) \quad (209)$$

$$\begin{pmatrix} \text{SG209} & a_1 & a_2 & a_3 \\ \nu & 12 & 8 & 6 \\ n_{\Gamma,1} & 1 & 1 & 1 \\ n_{\Gamma,2} & 1 & 1 & 0 \\ n_{\Gamma,3} & 2 & 1 & 1 \\ n_{X,1} & 3 & 2 & 2 \\ n_{X,2} & 3 & 2 & 1 \\ n_{L,1} & 2 & 1 & 1 \\ n_{L,2} & 2 & 1 & 1 \\ n_{L,3} & 4 & 3 & 2 \\ n_{W,1} & 6 & 4 & 3 \end{pmatrix} \quad (210)$$

$$\begin{pmatrix} \text{SG210} & a_1 & a_2 \\ \nu & 12 & 8 \\ n_{\Gamma,1} & 1 & 1 \\ n_{\Gamma,2} & 1 & 1 \\ n_{\Gamma,3} & 2 & 1 \\ n_{X,1} & 3 & 2 \\ n_{X,2} & 3 & 2 \\ n_{L,1} & 2 & 1 \\ n_{L,2} & 2 & 1 \\ n_{L,3} & 4 & 3 \\ n_{W,1} & 3 & 2 \\ n_{W,2} & 3 & 2 \\ n_{W,3} & 3 & 2 \\ n_{W,4} & 3 & 2 \end{pmatrix} \quad (211)$$

$$\begin{pmatrix} \text{SG211} & a_1 & a_2 & a_3 \\ \nu & 12 & 8 & 6 \\ n_{\Gamma,1} & 1 & 1 & 1 \\ n_{\Gamma,2} & 1 & 1 & 0 \\ n_{\Gamma,3} & 2 & 1 & 1 \\ n_{H,1} & 1 & 1 & 1 \\ n_{H,2} & 1 & 1 & 0 \\ n_{H,3} & 2 & 1 & 1 \\ n_{P,1} & 2 & 2 & 1 \\ n_{P,2} & 2 & 1 & 1 \\ n_{P,3} & 2 & 1 & 1 \\ n_{N,1} & 6 & 4 & 3 \end{pmatrix} \quad (212)$$

$$\left( \begin{array}{ccc} \text{SG212} & a_1 & a_2 \\ \nu & 24 & 8 \\ n_{\Gamma,1} & 2 & 1 \\ n_{\Gamma,2} & 2 & 1 \\ n_{\Gamma,3} & 4 & 1 \\ n_{X,1} & 3 & 1 \\ n_{X,2} & 3 & 1 \\ n_{X,3} & 3 & 1 \\ n_{X,4} & 3 & 1 \\ n_{X,5} & 6 & 2 \\ n_{M,1} & 6 & 2 \\ n_{M,2} & 6 & 2 \\ n_{R,1} & 1 & 0 \\ n_{R,2} & 1 & 0 \\ n_{R,3} & 2 & 1 \\ n_{R,4} & 3 & 1 \\ n_{R,5} & 3 & 1 \end{array} \right) \quad (213)$$

$$\left( \begin{array}{ccc} \text{SG213} & a_1 & a_2 \\ \nu & 24 & 8 \\ n_{\Gamma,1} & 2 & 1 \\ n_{\Gamma,2} & 2 & 1 \\ n_{\Gamma,3} & 4 & 1 \\ n_{X,1} & 3 & 1 \\ n_{X,2} & 3 & 1 \\ n_{X,3} & 3 & 1 \\ n_{X,4} & 3 & 1 \\ n_{X,5} & 6 & 2 \\ n_{M,1} & 6 & 2 \\ n_{M,2} & 6 & 2 \\ n_{R,1} & 1 & 0 \\ n_{R,2} & 1 & 0 \\ n_{R,3} & 2 & 1 \\ n_{R,4} & 3 & 1 \\ n_{R,5} & 3 & 1 \end{array} \right) \quad (214)$$

$$\left( \begin{array}{ccc} \text{SG214} & a_1 & a_2 \\ \nu & 12 & 8 \\ n_{\Gamma,1} & 1 & 1 \\ n_{\Gamma,2} & 1 & 1 \\ n_{\Gamma,3} & 2 & 1 \\ n_{H,1} & 1 & 1 \\ n_{H,2} & 1 & 1 \\ n_{H,3} & 2 & 1 \\ n_{P,1} & 1 & 0 \\ n_{P,2} & 1 & 1 \\ n_{P,3} & 1 & 1 \\ n_{P,4} & 3 & 2 \\ n_{N,1} & 6 & 4 \end{array} \right) \quad (215)$$

$$\left( \begin{array}{l} \text{SG215} \quad a_1 \quad a_2 \quad a_3 \quad a_4 \quad a_5 \quad a_6 \\ \nu \quad 12 \quad 4 \quad 6 \quad 6 \quad 2 \quad -12 \\ n_{\Gamma,1} \quad 1 \quad 0 \quad 1 \quad 1 \quad 1 \quad -2 \\ n_{\Gamma,2} \quad 1 \quad 0 \quad 0 \quad 0 \quad 0 \quad 0 \\ n_{\Gamma,3} \quad 2 \quad 1 \quad 1 \quad 1 \quad 0 \quad -2 \\ n_{X,1} \quad 3 \quad 1 \quad 2 \quad 1 \quad 1 \quad -4 \\ n_{X,2} \quad 3 \quad 1 \quad 1 \quad 2 \quad 0 \quad -2 \\ n_{M,1} \quad 3 \quad 1 \quad 1 \quad 2 \quad 1 \quad -4 \\ n_{M,2} \quad 3 \quad 1 \quad 2 \quad 1 \quad 0 \quad -2 \\ n_{R,1} \quad 1 \quad 0 \quad 1 \quad 1 \quad 0 \quad -2 \\ n_{R,2} \quad 1 \quad 0 \quad 0 \quad 0 \quad 1 \quad 0 \\ n_{R,3} \quad 2 \quad 1 \quad 1 \quad 1 \quad 0 \quad -2 \end{array} \right) \quad (216)$$

$$\left( \begin{array}{l} \text{SG216} \quad a_1 \quad a_2 \quad a_3 \quad a_4 \quad a_5 \quad a_6 \\ \nu \quad 12 \quad 4 \quad 2 \quad 2 \quad 2 \quad -4 \\ n_{\Gamma,1} \quad 1 \quad 0 \quad 1 \quad 1 \quad 1 \quad -2 \\ n_{\Gamma,2} \quad 1 \quad 0 \quad 0 \quad 0 \quad 0 \quad 0 \\ n_{\Gamma,3} \quad 2 \quad 1 \quad 0 \quad 0 \quad 0 \quad 0 \\ n_{X,1} \quad 3 \quad 1 \quad 1 \quad 1 \quad 0 \quad -2 \\ n_{X,2} \quad 3 \quad 1 \quad 0 \quad 0 \quad 1 \quad 0 \\ n_{L,1} \quad 2 \quad 1 \quad 0 \quad 0 \quad 0 \quad 0 \\ n_{L,2} \quad 2 \quad 1 \quad 0 \quad 0 \quad 0 \quad 0 \\ n_{L,3} \quad 4 \quad 1 \quad 1 \quad 1 \quad 1 \quad -2 \\ n_{W,1} \quad 3 \quad 1 \quad 0 \quad 1 \quad 1 \quad -2 \\ n_{W,2} \quad 3 \quad 1 \quad 0 \quad 1 \quad 0 \quad 0 \\ n_{W,3} \quad 3 \quad 1 \quad 1 \quad 0 \quad 0 \quad 0 \\ n_{W,4} \quad 3 \quad 1 \quad 1 \quad 0 \quad 1 \quad -2 \end{array} \right) \quad (217)$$

$$\left( \begin{array}{l} \text{SG217} \quad a_1 \quad a_2 \quad a_3 \quad a_4 \quad a_5 \\ \nu \quad 12 \quad 12 \quad 4 \quad 6 \quad -20 \\ n_{\Gamma,1} \quad 1 \quad 2 \quad 0 \quad 1 \quad -2 \\ n_{\Gamma,2} \quad 1 \quad 0 \quad 0 \quad 0 \quad 0 \\ n_{\Gamma,3} \quad 2 \quad 2 \quad 1 \quad 1 \quad -4 \\ n_{H,1} \quad 1 \quad 0 \quad 0 \quad 1 \quad 0 \\ n_{H,2} \quad 1 \quad 2 \quad 0 \quad 0 \quad -2 \\ n_{H,3} \quad 2 \quad 2 \quad 1 \quad 1 \quad -4 \\ n_{P,1} \quad 1 \quad 1 \quad 0 \quad 0 \quad 0 \\ n_{P,2} \quad 1 \quad 1 \quad 0 \quad 1 \quad -2 \\ n_{P,3} \quad 2 \quad 2 \quad 1 \quad 1 \quad -4 \\ n_{N,1} \quad 6 \quad 6 \quad 2 \quad 3 \quad -10 \end{array} \right) \quad (218)$$

$$\left( \begin{array}{l} \text{SG218} \quad a_1 \quad a_2 \quad a_3 \quad a_4 \\ \nu \quad 12 \quad 16 \quad 12 \quad 0 \\ n_{\Gamma,1} \quad 1 \quad 2 \quad 2 \quad 0 \\ n_{\Gamma,2} \quad 1 \quad 2 \quad 0 \quad 0 \\ n_{\Gamma,3} \quad 2 \quad 2 \quad 2 \quad 0 \\ n_{X,1} \quad 3 \quad 4 \quad 3 \quad 0 \\ n_{X,2} \quad 3 \quad 4 \quad 3 \quad 0 \\ n_{M,1} \quad 3 \quad 4 \quad 2 \quad 2 \\ n_{M,2} \quad 3 \quad 4 \quad 4 \quad -2 \\ n_{R,1} \quad 1 \quad 2 \quad 1 \quad 0 \\ n_{R,2} \quad 1 \quad 2 \quad 1 \quad 0 \\ n_{R,3} \quad 1 \quad 1 \quad 1 \quad 0 \end{array} \right) \quad (219)$$

$$\left( \begin{array}{ccccc} \text{SG219} & a_1 & a_2 & a_3 & a_4 \\ \nu & 12 & 16 & 12 & 0 \\ n_{\Gamma,1} & 1 & 2 & 2 & 0 \\ n_{\Gamma,2} & 1 & 2 & 0 & 0 \\ n_{\Gamma,3} & 2 & 2 & 2 & 0 \\ n_{X,1} & 3 & 4 & 2 & 2 \\ n_{X,2} & 3 & 4 & 4 & -2 \\ n_{L,1} & 1 & 1 & 1 & 0 \\ n_{L,2} & 1 & 1 & 1 & 0 \\ n_{L,3} & 2 & 3 & 2 & 0 \\ n_{W,1} & 3 & 4 & 3 & 0 \\ n_{W,2} & 3 & 4 & 3 & 0 \\ n_{W,3} & 3 & 4 & 3 & 0 \\ n_{W,4} & 3 & 4 & 3 & 0 \end{array} \right) \quad (220)$$

$$\left( \begin{array}{ccccc} \text{SG220} & a_1 & a_2 & a_3 & \\ \nu & 24 & 28 & -16 & \\ n_{\Gamma,1} & 2 & 3 & -2 & \\ n_{\Gamma,2} & 2 & 3 & -2 & \\ n_{\Gamma,3} & 4 & 4 & -2 & \\ n_{H,1} & 2 & 3 & -2 & \\ n_{H,2} & 2 & 3 & -2 & \\ n_{H,3} & 4 & 4 & -2 & \\ n_{P,1} & 1 & 1 & 0 & \\ n_{P,2} & 1 & 0 & 0 & \\ n_{P,3} & 2 & 3 & -2 & \\ n_{P,4} & 3 & 4 & -2 & \\ n_{P,5} & 3 & 3 & -2 & \\ n_{N,1} & 6 & 7 & -4 & \\ n_{N,2} & 6 & 7 & -4 & \\ n_{N,3} & 6 & 7 & -4 & \\ n_{N,4} & 6 & 7 & -4 & \end{array} \right) \quad (221)$$

$$\left( \begin{array}{l} \text{SG221} \quad a_1 \quad a_2 \quad a_3 \quad a_4 \quad a_5 \quad a_6 \quad a_7 \quad a_8 \quad a_9 \quad a_{10} \quad a_{11} \quad a_{12} \quad a_{13} \quad a_{14} \\ \nu \quad 24 \quad 8 \quad 12 \quad 12 \quad 6 \quad 6 \quad 6 \quad 6 \quad 2 \quad -44 \quad -78 \quad 2 \quad 144 \quad -64 \\ n_{\Gamma,1} \quad 1 \quad 0 \quad 1 \quad 1 \quad 1 \quad 0 \quad 1 \quad 0 \quad 1 \quad -6 \quad -9 \quad 1 \quad 16 \quad -8 \\ n_{\Gamma,2} \quad 1 \quad 0 \quad 0 \quad 0 \quad 0 \quad 1 \quad 0 \quad 1 \quad 0 \quad -4 \quad -6 \quad 0 \quad 12 \quad -8 \\ n_{\Gamma,3} \quad 2 \quad 1 \quad 0 \quad -6 \quad -9 \quad 0 \quad 16 \quad -8 \\ n_{\Gamma,4} \quad 1 \quad 0 \quad 1 \quad 1 \quad 0 \quad 0 \quad 0 \quad 0 \quad 0 \quad 0 \quad -2 \quad 0 \quad 4 \quad 0 \\ n_{\Gamma,5} \quad 1 \quad 0 \\ n_{\Gamma,6} \quad 2 \quad 1 \quad 1 \quad 1 \quad 0 \quad 0 \quad 0 \quad 0 \quad 0 \quad 0 \quad -2 \quad 0 \quad 4 \quad 0 \\ n_{X,1} \quad 3 \quad 1 \quad 2 \quad 2 \quad 1 \quad 1 \quad 1 \quad 0 \quad 0 \quad -6 \quad -11 \quad 1 \quad 20 \quad -8 \\ n_{X,2} \quad 3 \quad 1 \quad 1 \quad 1 \quad 1 \quad 1 \quad 0 \quad 1 \quad 0 \quad -5 \quad -8 \quad 0 \quad 16 \quad -8 \\ n_{X,3} \quad 3 \quad 1 \quad 2 \quad 2 \quad 1 \quad 0 \quad 1 \quad 1 \quad 1 \quad -6 \quad -11 \quad 0 \quad 20 \quad -8 \\ n_{X,4} \quad 3 \quad 1 \quad 1 \quad 1 \quad 0 \quad 1 \quad 1 \quad 1 \quad 0 \quad -5 \quad -9 \quad 0 \quad 16 \quad -8 \\ n_{M,1} \quad 3 \quad 1 \quad 1 \quad 2 \quad 1 \quad 0 \quad 0 \quad 1 \quad 0 \quad -5 \quad -9 \quad 1 \quad 16 \quad -8 \\ n_{M,2} \quad 3 \quad 1 \quad 2 \quad 1 \quad 0 \quad 1 \quad 1 \quad 0 \quad 1 \quad -5 \quad -8 \quad 0 \quad 16 \quad -8 \\ n_{M,3} \quad 3 \quad 1 \quad 1 \quad 2 \quad 1 \quad 1 \quad 1 \quad 1 \quad 0 \quad -6 \quad -11 \quad 0 \quad 20 \quad -8 \\ n_{M,4} \quad 3 \quad 1 \quad 2 \quad 1 \quad 1 \quad 1 \quad 1 \quad 1 \quad 0 \quad -6 \quad -11 \quad 0 \quad 20 \quad -8 \\ n_{R,1} \quad 1 \quad 0 \quad 0 \quad 1 \quad 0 \quad 0 \quad 0 \quad 1 \quad 0 \quad -5 \quad -7 \quad 1 \quad 12 \quad -8 \\ n_{R,2} \quad 1 \quad 0 \quad 1 \quad 0 \quad 0 \quad 0 \quad 1 \quad 0 \quad 0 \quad 0 \quad -2 \quad 0 \quad 4 \quad 0 \\ n_{R,3} \quad 2 \quad 1 \quad 1 \quad 1 \quad 0 \quad 0 \quad 1 \quad 1 \quad 0 \quad -1 \quad -5 \quad 0 \quad 8 \quad 0 \\ n_{R,4} \quad 1 \quad 0 \quad 0 \quad 1 \quad 1 \quad 0 \quad 0 \quad 0 \quad 0 \quad 0 \quad -2 \quad 0 \quad 4 \quad 0 \\ n_{R,5} \quad 1 \quad 0 \quad 1 \quad 0 \quad 0 \quad 1 \quad 0 \quad 0 \quad 1 \quad -5 \quad -6 \quad 0 \quad 12 \quad -8 \\ n_{R,6} \quad 2 \quad 1 \quad 1 \quad 1 \quad 1 \quad 1 \quad 0 \quad 0 \quad 0 \quad -5 \quad -6 \quad 0 \quad 12 \quad -8 \end{array} \right) \quad (222)$$

$$\left( \begin{array}{l} \text{SG222} \quad a_1 \quad a_2 \quad a_3 \quad a_4 \quad a_5 \quad a_6 \\ \nu \quad 24 \quad 16 \quad 12 \quad 24 \quad 16 \quad -64 \\ n_{\Gamma,1} \quad 1 \quad 1 \quad 1 \quad 2 \quad 2 \quad -8 \\ n_{\Gamma,2} \quad 1 \quad 1 \quad 0 \quad 0 \quad 2 \quad -4 \\ n_{\Gamma,3} \quad 2 \quad 1 \quad 1 \quad 2 \quad 2 \quad -4 \\ n_{\Gamma,4} \quad 1 \quad 1 \quad 1 \quad 0 \quad 0 \quad 0 \\ n_{\Gamma,5} \quad 1 \quad 1 \quad 0 \quad 2 \quad 0 \quad -4 \\ n_{\Gamma,6} \quad 2 \quad 1 \quad 1 \quad 2 \quad 0 \quad -4 \\ n_{X,1} \quad 3 \quad 2 \quad 2 \quad 3 \quad 2 \quad -8 \\ n_{X,2} \quad 3 \quad 2 \quad 2 \quad 3 \quad 2 \quad -8 \\ n_{X,3} \quad 3 \quad 2 \quad 1 \quad 3 \quad 2 \quad -8 \\ n_{X,4} \quad 3 \quad 2 \quad 1 \quad 3 \quad 2 \quad -8 \\ n_{M,1} \quad 6 \quad 4 \quad 3 \quad 6 \quad 4 \quad -16 \\ n_{R,1} \quad 2 \quad 2 \quad 1 \quad 2 \quad 2 \quad -8 \\ n_{R,2} \quad 2 \quad 1 \quad 1 \quad 2 \quad 1 \quad -4 \\ n_{R,3} \quad 2 \quad 1 \quad 1 \quad 2 \quad 1 \quad -4 \end{array} \right) \quad (223)$$

$$\left( \begin{array}{ccccccccc} \text{SG223} & a_1 & a_2 & a_3 & a_4 & a_5 & a_6 & a_7 \\ \nu & 24 & 16 & 12 & 12 & 12 & 4 & -64 \\ n_{\Gamma,1} & 1 & 1 & 1 & 1 & 1 & 1 & -8 \\ n_{\Gamma,2} & 1 & 1 & 0 & 0 & 1 & 1 & -4 \\ n_{\Gamma,3} & 2 & 1 & 1 & 1 & 2 & 0 & -4 \\ n_{\Gamma,4} & 1 & 1 & 0 & 0 & 0 & 0 & 0 \\ n_{\Gamma,5} & 1 & 1 & 1 & 1 & 0 & 0 & -4 \\ n_{\Gamma,6} & 2 & 1 & 1 & 1 & 0 & 0 & -4 \\ n_{X,1} & 6 & 4 & 3 & 3 & 3 & 1 & -16 \\ n_{M,1} & 3 & 2 & 2 & 1 & 1 & 1 & -8 \\ n_{M,2} & 3 & 2 & 1 & 2 & 1 & 1 & -8 \\ n_{M,3} & 3 & 2 & 1 & 2 & 2 & 0 & -8 \\ n_{M,4} & 3 & 2 & 2 & 1 & 2 & 0 & -8 \\ n_{R,1} & 2 & 2 & 1 & 1 & 1 & 1 & -8 \\ n_{R,2} & 2 & 1 & 1 & 1 & 1 & 0 & -4 \\ n_{R,3} & 2 & 1 & 1 & 1 & 1 & 0 & -4 \end{array} \right) \quad (224)$$

$$\left( \begin{array}{ccccccccc} \text{SG224} & a_1 & a_2 & a_3 & a_4 & a_5 & a_6 & a_7 & a_8 \\ \nu & 24 & 8 & 12 & -32 & 8 & -64 & 72 & -80 \\ n_{\Gamma,1} & 1 & 0 & 1 & -2 & 1 & -3 & 4 & -4 \\ n_{\Gamma,2} & 1 & 0 & 0 & -2 & 1 & -3 & 4 & -4 \\ n_{\Gamma,3} & 2 & 1 & 1 & -4 & 1 & -9 & 10 & -12 \\ n_{\Gamma,4} & 1 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ n_{\Gamma,5} & 1 & 0 & 1 & 0 & 0 & 0 & 0 & 0 \\ n_{\Gamma,6} & 2 & 1 & 1 & -2 & 0 & -4 & 4 & -4 \\ n_{X,1} & 6 & 2 & 3 & -8 & 2 & -16 & 18 & -20 \\ n_{M,1} & 6 & 2 & 3 & -8 & 2 & -16 & 18 & -20 \\ n_{R,1} & 1 & 0 & 0 & 0 & 0 & 1 & 0 & 0 \\ n_{R,2} & 1 & 0 & 1 & -2 & 0 & -3 & 4 & -4 \\ n_{R,3} & 2 & 1 & 1 & -3 & 0 & -5 & 6 & -8 \\ n_{R,4} & 1 & 0 & 1 & -2 & 1 & -4 & 4 & -4 \\ n_{R,5} & 1 & 0 & 0 & 0 & 1 & 0 & 0 & 0 \\ n_{R,6} & 2 & 1 & 1 & -3 & 1 & -8 & 8 & -8 \end{array} \right) \quad (225)$$

$$\left( \begin{array}{cccccccccccc} \text{SG225} & a_1 & a_2 & a_3 & a_4 & a_5 & a_6 & a_7 & a_8 & a_9 & a_{10} & a_{11} \\ \nu & 24 & 8 & 12 & 12 & 4 & 2 & 2 & 4 & 2 & -130 & -256 \\ n_{\Gamma,1} & 1 & 0 & 1 & 1 & 1 & 1 & 0 & 0 & 1 & -13 & -24 \\ n_{\Gamma,2} & 1 & 0 & 0 & 1 & 0 & 0 & 1 & 0 & 0 & -4 & -8 \\ n_{\Gamma,3} & 2 & 1 & 1 & 2 & 0 & 0 & 0 & 1 & 0 & -12 & -24 \\ n_{\Gamma,4} & 1 & 0 & 1 & 0 & 0 & 0 & 0 & 0 & 0 & -4 & -8 \\ n_{\Gamma,5} & 1 & 0 & 0 & 0 & 1 & 0 & 0 & 0 & 0 & -4 & -8 \\ n_{\Gamma,6} & 2 & 1 & 1 & 0 & 0 & 0 & 0 & 0 & 0 & -8 & -16 \\ n_{X,1} & 3 & 1 & 2 & 1 & 0 & 1 & 0 & 1 & 1 & -21 & -40 \\ n_{X,2} & 3 & 1 & 1 & 1 & 1 & 0 & 1 & 1 & 0 & -16 & -32 \\ n_{X,3} & 3 & 1 & 2 & 2 & 1 & 0 & 0 & 0 & 0 & -16 & -32 \\ n_{X,4} & 3 & 1 & 1 & 2 & 0 & 0 & 0 & 0 & 0 & -12 & -24 \\ n_{L,1} & 2 & 1 & 1 & 1 & 0 & 0 & 0 & 0 & 0 & -8 & -16 \\ n_{L,2} & 2 & 1 & 1 & 1 & 0 & 0 & 0 & 0 & 0 & -8 & -16 \\ n_{L,3} & 4 & 1 & 2 & 2 & 1 & 0 & 0 & 0 & 1 & -20 & -40 \\ n_{L,4} & 2 & 1 & 1 & 1 & 0 & 0 & 0 & 1 & 0 & -12 & -24 \\ n_{L,5} & 2 & 1 & 1 & 1 & 0 & 0 & 0 & 1 & 0 & -12 & -24 \\ n_{L,6} & 4 & 1 & 2 & 2 & 1 & 1 & 1 & 1 & 0 & -25 & -48 \\ n_{W,1} & 6 & 2 & 3 & 3 & 1 & 1 & 0 & 1 & 0 & -32 & -64 \\ n_{W,2} & 6 & 2 & 3 & 3 & 1 & 0 & 1 & 1 & 1 & -33 & -64 \end{array} \right) \quad (226)$$

$$\left( \begin{array}{l} \text{SG226} \\ \nu \quad 24 \quad 16 \quad 12 \quad 12 \quad -112 \quad 12 \quad 4 \quad -224 \\ n_{\Gamma,1} \quad 1 \quad 1 \quad 1 \quad 2 \quad -9 \quad 1 \quad 1 \quad -16 \\ n_{\Gamma,2} \quad 1 \quad 1 \quad 0 \quad 0 \quad -7 \quad 0 \quad 1 \quad -16 \\ n_{\Gamma,3} \quad 2 \quad 1 \quad 1 \quad 2 \quad -8 \quad 1 \quad 0 \quad -16 \\ n_{\Gamma,4} \quad 1 \quad 1 \quad 1 \quad 0 \quad -4 \quad 0 \quad 0 \quad -8 \\ n_{\Gamma,5} \quad 1 \quad 1 \quad 0 \quad 0 \quad -4 \quad 1 \quad 0 \quad -8 \\ n_{\Gamma,6} \quad 2 \quad 1 \quad 1 \quad 0 \quad -8 \quad 1 \quad 0 \quad -16 \\ n_{X,1} \quad 3 \quad 2 \quad 2 \quad 2 \quad -13 \quad 1 \quad 1 \quad -24 \\ n_{X,2} \quad 3 \quad 2 \quad 1 \quad 0 \quad -15 \quad 2 \quad 1 \quad -32 \\ n_{X,3} \quad 3 \quad 2 \quad 2 \quad 2 \quad -16 \quad 2 \quad 0 \quad -32 \\ n_{X,4} \quad 3 \quad 2 \quad 1 \quad 2 \quad -12 \quad 1 \quad 0 \quad -24 \\ n_{L,1} \quad 2 \quad 1 \quad 1 \quad 1 \quad -8 \quad 1 \quad 0 \quad -16 \\ n_{L,2} \quad 4 \quad 3 \quad 2 \quad 2 \quad -20 \quad 2 \quad 1 \quad -40 \\ n_{L,3} \quad 4 \quad 3 \quad 2 \quad 2 \quad -20 \quad 2 \quad 1 \quad -40 \\ n_{W,1} \quad 6 \quad 4 \quad 3 \quad 3 \quad -28 \quad 3 \quad 1 \quad -56 \\ n_{W,2} \quad 6 \quad 4 \quad 3 \quad 3 \quad -28 \quad 3 \quad 1 \quad -56 \end{array} \right) \quad (227)$$

$$\left( \begin{array}{l} \text{SG227} \\ \nu \quad 24 \quad 8 \quad 8 \quad 8 \quad -24 \quad 8 \quad 4 \quad -48 \\ n_{\Gamma,1} \quad 1 \quad 0 \quad 0 \quad 1 \quad -2 \quad 1 \quad 1 \quad -4 \\ n_{\Gamma,2} \quad 1 \quad 0 \quad 0 \quad 1 \quad -2 \quad 1 \quad 0 \quad -4 \\ n_{\Gamma,3} \quad 2 \quad 1 \quad 2 \quad 1 \quad -4 \quad 1 \quad 0 \quad -8 \\ n_{\Gamma,4} \quad 1 \quad 0 \\ n_{\Gamma,5} \quad 1 \quad 0 \quad 0 \quad 0 \quad 0 \quad 0 \quad 1 \quad 0 \\ n_{\Gamma,6} \quad 2 \quad 1 \quad 0 \quad 0 \quad 0 \quad 0 \quad 0 \quad 0 \\ n_{X,1} \quad 6 \quad 2 \quad 2 \quad 2 \quad -6 \quad 2 \quad 1 \quad -12 \\ n_{L,1} \quad 2 \quad 1 \quad 1 \quad 1 \quad -2 \quad 0 \quad 0 \quad -4 \\ n_{L,2} \quad 2 \quad 1 \quad 1 \quad 1 \quad -2 \quad 0 \quad 0 \quad -4 \\ n_{L,3} \quad 4 \quad 1 \quad 2 \quad 2 \quad -5 \quad 1 \quad 1 \quad -8 \\ n_{L,4} \quad 2 \quad 1 \quad 1 \quad 0 \quad -2 \quad 1 \quad 0 \quad -4 \\ n_{L,5} \quad 2 \quad 1 \quad 1 \quad 0 \quad -2 \quad 1 \quad 0 \quad -4 \\ n_{L,6} \quad 4 \quad 1 \quad 0 \quad 1 \quad -3 \quad 2 \quad 1 \quad -8 \\ n_{W,1} \quad 3 \quad 1 \quad 1 \quad 1 \quad -2 \quad 1 \quad 0 \quad -4 \\ n_{W,2} \quad 3 \quad 1 \quad 1 \quad 1 \quad -2 \quad 1 \quad 0 \quad -4 \\ n_{W,3} \quad 3 \quad 1 \quad 1 \quad 1 \quad -4 \quad 1 \quad 1 \quad -8 \\ n_{W,4} \quad 3 \quad 1 \quad 1 \quad 1 \quad -4 \quad 1 \quad 1 \quad -8 \\ n_{W,5} \quad 6 \quad 2 \quad 2 \quad 2 \quad -6 \quad 2 \quad 1 \quad -12 \end{array} \right) \quad (228)$$

$$\left( \begin{array}{cccccc} \text{SG228} & a_1 & a_2 & a_3 & a_4 & a_5 \\ \nu & 24 & 16 & 24 & 16 & -64 \\ n_{\Gamma,1} & 1 & 1 & 2 & 2 & -8 \\ n_{\Gamma,2} & 1 & 1 & 0 & 2 & -4 \\ n_{\Gamma,3} & 2 & 1 & 2 & 2 & -4 \\ n_{\Gamma,4} & 1 & 1 & 0 & 0 & 0 \\ n_{\Gamma,5} & 1 & 1 & 2 & 0 & -4 \\ n_{\Gamma,6} & 2 & 1 & 2 & 0 & -4 \\ n_{X,1} & 6 & 4 & 6 & 4 & -16 \\ n_{L,1} & 2 & 1 & 2 & 1 & -4 \\ n_{L,2} & 4 & 3 & 4 & 3 & -12 \\ n_{L,3} & 4 & 3 & 4 & 3 & -12 \\ n_{W,1} & 3 & 2 & 3 & 2 & -8 \\ n_{W,2} & 3 & 2 & 3 & 2 & -8 \\ n_{W,3} & 3 & 2 & 3 & 2 & -8 \\ n_{W,4} & 3 & 2 & 3 & 2 & -8 \\ n_{W,5} & 3 & 2 & 3 & 2 & -8 \end{array} \right) \quad (229)$$

$$\left( \begin{array}{cccccccccccc} \text{SG229} & a_1 & a_2 & a_3 & a_4 & a_5 & a_6 & a_7 & a_8 & a_9 & a_{10} & a_{11} \\ \nu & 24 & 8 & 12 & 12 & -360 & 8 & 6 & 6 & 2 & 204 & -256 \\ n_{\Gamma,1} & 1 & 0 & 1 & 1 & -34 & 1 & 1 & 0 & 1 & 18 & -24 \\ n_{\Gamma,2} & 1 & 0 & 0 & 0 & -10 & 1 & 0 & 1 & 0 & 4 & -8 \\ n_{\Gamma,3} & 2 & 1 & 1 & 1 & -32 & 1 & 1 & 1 & 0 & 16 & -24 \\ n_{\Gamma,4} & 1 & 0 & 1 & 0 & -12 & 0 & 0 & 0 & 0 & 8 & -8 \\ n_{\Gamma,5} & 1 & 0 & 0 & 1 & -12 & 0 & 0 & 0 & 0 & 8 & -8 \\ n_{\Gamma,6} & 2 & 1 & 1 & 1 & -24 & 0 & 0 & 0 & 0 & 16 & -16 \\ n_{H,1} & 1 & 0 & 1 & 0 & -23 & 0 & 1 & 0 & 1 & 12 & -16 \\ n_{H,2} & 1 & 0 & 0 & 1 & -11 & 0 & 0 & 1 & 0 & 6 & -8 \\ n_{H,3} & 2 & 1 & 1 & 1 & -23 & 0 & 1 & 1 & 0 & 12 & -16 \\ n_{H,4} & 1 & 0 & 1 & 1 & -23 & 1 & 0 & 0 & 0 & 14 & -16 \\ n_{H,5} & 1 & 0 & 0 & 0 & -11 & 1 & 0 & 0 & 0 & 6 & -8 \\ n_{H,6} & 2 & 1 & 1 & 1 & -33 & 1 & 0 & 0 & 0 & 20 & -24 \\ n_{P,1} & 2 & 0 & 1 & 1 & -34 & 1 & 1 & 0 & 0 & 20 & -24 \\ n_{P,2} & 2 & 0 & 1 & 1 & -34 & 1 & 0 & 1 & 1 & 18 & -24 \\ n_{P,3} & 4 & 2 & 2 & 2 & -56 & 1 & 1 & 1 & 0 & 32 & -40 \\ n_{N,1} & 6 & 2 & 3 & 3 & -90 & 2 & 1 & 1 & 1 & 52 & -64 \\ n_{N,2} & 6 & 2 & 3 & 3 & -90 & 2 & 2 & 2 & 0 & 50 & -64 \end{array} \right) \quad (230)$$

	SG230	$a_1$	$a_2$	$a_3$	$a_4$	$a_5$	
$\nu$	24	16	24	16	-64		
$n_{\Gamma,1}$	1	1	2	2	-8		
$n_{\Gamma,2}$	1	1	0	2	-4		
$n_{\Gamma,3}$	2	1	2	2	-4		
$n_{\Gamma,4}$	1	1	0	0	0		
$n_{\Gamma,5}$	1	1	2	0	-4		
$n_{\Gamma,6}$	2	1	2	0	-4		
$n_{H,1}$	2	2	2	2	-8		
$n_{H,2}$	2	1	2	1	-4		
$n_{H,3}$	2	1	2	1	-4		
$n_{P,1}$	1	0	1	0	0		
$n_{P,2}$	1	0	1	0	0		
$n_{P,3}$	2	2	2	2	-8		
$n_{P,4}$	3	2	3	2	-8		
$n_{P,5}$	3	2	3	2	-8		
$n_{N,1}$	6	4	6	4	-16		
$n_{N,2}$	6	4	6	4	-16		

(231)

## VI. WEBSITE FOR BAND STRUCTURES

The band structures computed for all of the discovered topological materials candidates can be found on the following website:

[ccmp.nju.edu.cn](http://ccmp.nju.edu.cn)

While the materials are grouped by their topological diagnosis and space groups, the database is also searchable. However, in searching one has to pay special attention to the naming convention adopted. For instance, the entry for Na<sub>3</sub>Bi can be found by any one of the following search prompts:

- “Bi1Na3”
- “Bi Na”
- “Na Bi”

Note, however, the prompts “Na3Bi”, “Na3Bi1”, and “BiNa3” will not return the correct result.

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