Supplementary Information for
"Classification of second harmonic generation effect in magnetic materials"

Rui-Chun Xiao,[*] Ding-Fu Shao, Wei Gan, Huan-Wen Wang, Hui Han, Z. G. Sheng, Changjin Zhang, Hua Jiang,[†] and Hui Li[‡]

Contents

---

*Electronic address: xiaoruichun@ahu.edu.cn
†Electronic address: jianghuaphy@suda.edu.cn
‡Electronic address: huili@ahu.edu.cn

Supplementary Note 1. SYMMETRY OF SHG TENSORS USING ISOMORPHIC GROUP METHOD

Suppl. Note 1.1. Profile of SHG effect

In a crystal, the electric polarization **P** can be expressed as a Taylor expansion of the macroscopic electric field **E**

$$\mathbf{P} = \varepsilon_0 \boldsymbol{\chi}^{(1)}(\omega) \cdot \mathbf{E} + \boldsymbol{\chi}^{(2)}(2\omega) : \mathbf{EE} + \cdots , \tag{S1}$$

where the $\boldsymbol{\chi}^{(1)}$ and $\boldsymbol{\chi}^{(2)}$ are second-rank ($[\chi^{(1)}_{ij}]_{3\times3}$) and third-rank ($[\chi^{(2)}_{ijk}]_{3\times3\times3}$) tensors, corresponding to linear and nonlinear (SHG) optical susceptibilities, respectively. Since the electric field **E** and polarization **P** are all odd under inversion symmetry P, the SHG tensor $\boldsymbol{\chi}^{(2)}$ only exists in P-breaking materials, according to Eq. (S1). For nonmagnetic materials, the breaking of inversion symmetry is induced by the crystal structure asymmetry. While for magnetic materials, the orderly arranged magnetic moments of atoms can also break the inversion symmetry and lead to the SHG effect.

The SHG susceptibilities $\chi^{(2)}_{abc,i}(\omega)$ are numerically calculated by [1–3]

$$\chi^{(2)}_{abc}(\omega) = \chi^{(2)}_{abc,e}(\omega) + \chi^{(2)}_{abc,i}(\omega), \tag{S2}$$

where the first one is a pure interband term

$$\begin{aligned}\chi^{(2)}_{abc,e}(\omega) = \frac{e^3}{2\hbar^2} {\sum_{nml}}' \int \frac{d^3\mathbf{k}}{(2\pi)^3} \frac{r^a_{nm}\left(r^b_{ml} r^c_{ln} + r^c_{ml} r^b_{ln}\right)}{\omega_{ln} - \omega_{ml}} \\ \times \left[\frac{2 f_{nm}}{\omega_{mn} - 2\omega} + \frac{f_{ln}}{\omega_{ln} - \omega} + \frac{f_{ml}}{\omega_{ml} - \omega}\right].\end{aligned} \tag{S3}$$

$\sum'$ in Eq. (S3) means that band indices n, m, l are not equal to each other in the summation. The second term in Eq. (S2) is a mixed band term, and

$$\begin{aligned}&\chi^{(2)}_{abc,i}(\omega) = \frac{ie^3}{2\hbar^2} \sum_{nm} f_{nm} \int \frac{d^3\mathbf{k}}{(2\pi)^3} \times \\ &[\frac{2 r^a_{nm}\left(r^b_{mn;c} + r^c_{mn;b}\right)}{\omega_{mn}\left(\omega_{mn} - 2\omega\right)} + \frac{r^a_{nm;c} r^b_{mn} + r^a_{nm;b} r^c_{mn}}{\omega_{mn}\left(\omega_{mn} - \omega\right)} \\ &+ \frac{r^a_{nm}\left(r^b_{mn}\Delta^c_{mn} + r^c_{mn}\Delta^b_{mn}\right)}{\omega^2_{mn}} \left(\frac{1}{\omega_{mn} - \omega} - \frac{4}{\omega_{mn} - 2\omega}\right) \\ &- \frac{r^b_{nm;a} r^c_{mn} + r^c_{nm;a} r^b_{mn}}{2\omega_{mn}\left(\omega_{mn} - \omega\right)} - \frac{\Delta^a_{mn} \operatorname{Re}(r^b_{nm} r^c_{mn})}{2\omega^2_{mn}\left(\omega_{mn} - \omega\right)}]\end{aligned} \tag{S4}$$

where ω is short for $\omega + i\delta$ ($\delta = \hbar/\tau$, where τ is the quasi-particle lifetime).

Suppl. Note 1.2. Brief introduction of magnetic groups

Since the symmetries of SHG are constrained by the magnetic groups, we introduce magnetic space groups (MSGs, also called Shubnikov groups) and magnetic point groups (MPGs) [4–6] briefly. In addition to the three-dimensional (3D) spatial symmetry operations $\{R|\mathbf{t}_0\}$ (named the unitary symmetry operations. R is the point operation, and $\mathbf{t}_0$ is the translation operator), MSGs also have the symmetry operations that contain time-reversal symmetry $\{R|\mathbf{t}_0\}'$ ($\{R|\mathbf{t}_0\}' = \{R|\mathbf{t}_0\} \cdot T$, named anti-unitary symmetry operation as T is an anti-unitary operator), which transform the position of atoms and then reverse the magnetic moments.

Suppl. Tab. I: Types of magnetic space groups (MSGs) and magnetic point groups (MPGs).

<table>
<tr><th>MSG M</th><th>Description</th><th>Number</th><th>Corresponding MPG M_0</th></tr>
<tr><td>Type-I Original MSG</td><td>$M = G$</td><td>230</td><td>Original MPG (32)
M_0=G_0</td></tr>
<tr><td>Type-II Grey MSG</td><td>$M = G + TG$</td><td>230</td><td rowspan="2">Grey MPG (32)
$M_0 = G_0 + TG_0$</td></tr>
<tr><td>Type-IV BW MSG
(BW Bravais lattices)</td><td>$M = G + T\{E \mid \mathbf{t}_0\}G$
($\mathbf{t}_0$ is half a unit cell translation)</td><td>517</td></tr>
<tr><td>Type-III BW MSG
(ordinary Bravais lattices)</td><td>$M = S + T(G - S)$</td><td>674</td><td>BW MPG (58)
$M_0 = S_0 + T(G_0 - S_0) = S_0 + R'S_0$</td></tr>
</table>

1 G and G_0 indicate the nonmagnetic space group (SG) and point group (PG), M and M_0 represent MSG and MPG, respectively.
2 The numbers in brackets in the fourth column indicate the amount of MPGs.
3 S_0 is the invariant subgroup of point group G_0 ($s = g/2$, s and g are the orders of S_0 and G_0, respectively).
4 R' is cosset represent element of set $R'H_0$, and R can be C_2, m, I, C_4, S_4, C_6 and S_6 whose symmetry order are even numbers.

The 1651 MSGs and 122 MPGs can be constructed by 230 nonmagnetic space groups (SGs) and 32 non-magnetic point groups (PGs), as listed in Table I. The MSGs can be divided into 4 types [4–6]. The type-I original (or colorless) MSGs have no anti-unitary operation. Type-II grey MSGs have both unitary operation $\{R|\mathbf{t}_0\}$ and corresponding anti-unitary operation $\{R|\mathbf{t}_0\}'$. The description of this kind of MSGs is $M = G+TG$, and they can be used to describe the nonmagnetic materials and parent phases (above the magnetic transition temperature) of magnetic materials. The type-IV black-white (BW) MSGs have anti-unitary operations of $T \cdot \{E \mid \mathbf{t}_0\}$ [$\mathbf{t}_0 = 1/2(n_1\mathbf{a}_1 + n_2\mathbf{a}_2 + n_3\mathbf{a}_3)$, ($n_i = 0$ or $1,\ i = 1, 2, 3$)], and they lead to these MSGs with BW Bravais lattices. Because the anti-unitary operations $\{R|\mathbf{t}_0\}'$ have the half lattice translations $\mathbf{t_0}$, the corresponding point groups of type-IV MPGs are grey MPGs, same as type-II MPGs. The type-III BW MSGs are expressed by $M = S + T(G - S)$, i.e., MSGs M are constructed by isomorphic space group G, invariant subgroup S, and $T(G - S)$.

Suppl. Note 1.3. Symmetry constraint of SHG tensor under magnetic symmetry operation

The expression of SHG tensor $\chi^{(2)}_{ijk}$ is calculated by Eq. (S2)-(S4), and can be simply expressed by

$$\chi^{(2)}_{ijk} \propto \int \frac{A}{\omega_{mn} - \eta\omega - i\hbar/\tau} d[\mathbf{k}], \tag{S5}$$

where A is a complex number ($A = \mathrm{Re}\,A + i\,\mathrm{Im}\,A$), and η =1 or 2. The real part of A is invariant under the time-reversal operation T, while the imaginary part reverses with T. Therefore, we can divide the SHG tensor into T-even (i-type) and T-odd (c-type) parts,

$$\chi^{(2)}_{ijk} = \chi^{\mathrm{even}}_{ijk} + \chi^{\mathrm{odd}}_{ijk}. \tag{S6}$$

According to Neumann principle [7–10], the symmetries of the SHG tensors are constrained by the MPGs M_0. The transformations of the even and odd part of SHG under the unitary operation are

$$R : \chi_{ijk}^{\text{even/odd}} = \sum_{lmn} R_{il} R_{jm} R_{kn} \chi_{lmn}^{\text{even/odd}}, \tag{S7}$$

where R_{ij} is the element of the 3×3 matrix of the point-group operation R. According to Eq. (S7), the transformations of χ_{ijk}^{even} and χ_{ijk}^{odd} are the same under unitary symmetry R, since R does not contain time operation. However, χ_{ijk}^{even} and χ_{ijk}^{odd} are different under the anti-unitary operation R' ($R' = TR$)

$$R' : \chi_{ijk}^{\text{even/odd}} = \pm \sum_{lmn} R_{il} R_{jm} R_{kn} \chi_{lmn}^{\text{even/odd}}. \tag{S8}$$

The plus and minus sign in Eq. (S8) correspond to the even part (χ_{ijk}^{even}) and the odd part (χ_{ijk}^{odd}) of SHG, respectively, which satisfy the Onsager reciprocal relation [9]. The transformation of χ_{ijk}^{even} under R' [Eq. (S8)] is equivalent to R [Eq. (S7)]. While a minus sign emerges when χ_{ijk}^{odd} is transformed under an anti-unitary operation R'.

Suppl. Note 1.4. Symmetry of SHG in MPGs with isomorphic group method

Numerically solving Eq. (S7) and Eq. (S8) directly, we can obtain the symmetries of SHG in all MPGs, as Refs. [7–9]. However, to capture the relationships between MPGs and SHG tensors and the rules of SHG tensors symmetries under all MPGs clearly, we study the symmetries of SHG via the isomorphic group method as follows. Because $-1 = -(I_0)_{3\times3}$ (I_0 is the identity matrix), i.e., -1 is identical to the matrix of inversion symmetry I, the transformation of χ_{ijk}^{odd} of Eq. (S8) under the anti-unitary operation R' can be re-written as

$$\begin{aligned} R' : \chi_{ijk}^{\text{odd}} &= -\sum_{lmn} R_{il} R_{jm} R_{kn} \chi_{lmn}^{\text{odd}} \\ &= \sum_{lmn} (-R)_{il} (-R)_{jm} (-R)_{kn} \chi_{lmn}^{\text{odd}} \\ &= \sum_{lmn} (IR)_{il} (IR)_{jm} (IR)_{kn} \chi_{lmn}^{\text{odd}}. \end{aligned} \tag{S9}$$

As can be seen, the constraint of anti-unitary operation R' on χ_{ijk}^{odd} is equivalent to a unitary operation IR. As summarized in Fig. 1 of the main text, we can use G_0 and its isomorphic group $G_1 = S_0 + IRS_0$ to seek the symmetry of the even (χ_{ijk}^{even}) and odd (χ_{ijk}^{odd}) parts of SHG, respectively. In other words, this method can transform the SHG symmetries under MPGs into nonmagnetic PGs.

In the following, we will study the symmetries of SHG of all MPGs with the isomorphic group method.

(1) Original MPGs $M_0 = G_0$. Since there is no anti-unitary symmetry operation in original MPGs, χ_{ijk}^{even} and χ_{ijk}^{odd} have the same symmetry constraint according to Eq. (S7), leading to χ_{ijk}^{even} and χ_{ijk}^{odd} possess the same tensor forms. The symmetries of SHG tensors under original MPGs can be obtained by Eq. (S7), besides they can also be found in general nonlinear optics textbooks [11, 12], and are also shown in Table IV of Supplementary Note 3. Because χ_{ijk}^{even} and χ_{ijk}^{odd} mix together, the SHG tensor elements cannot be described by the c-type or i-type simply, as claimed in the introduction part of main text. Since time-reversal operator T reverses χ_{ijk}^{odd}, and keep χ_{ijk}^{even} invariant, therefore we can distinguish them by reversing all the magnetic moments in the theoretical calculations, then

$$\begin{cases} \chi_{ijk}^{\text{even}}([\mathbf{M}]) = \left[\chi_{ijk}^{(2)}([\mathbf{M}]) + \chi_{ijk}^{(2)}([-\mathbf{M}])\right]/2, \\ \chi_{ijk}^{\text{odd}}([\mathbf{M}]) = \left[\chi_{ijk}^{(2)}([\mathbf{M}]) - \chi_{ijk}^{(2)}([-\mathbf{M}])\right]/2, \end{cases} \tag{S10}$$

where $\chi_{ijk}^{(2)}$ is the calculated SHG susceptibility, and $[\mathbf{M}] = [\mathbf{M}_A, \mathbf{M}_B, \ldots]$ denotes the directions of all magnetic moments in the unit cell.

(2) Grey MPGs $M_0 = G_0 + TG_0$. In grey MPGs, a unitary operation R must correspond to an anti-unitary operation R'. According to Eq. (S7) and Eq. (S8), the transformations of χ_{ijk}^{odd} under R and R' are

$$\begin{cases} R : \chi_{ijk}^{\text{odd}} = \sum\limits_{lmn} R_{il} R_{jm} R_{kn} \chi_{lmn}^{\text{odd}}, \\ R' : \chi_{ijk}^{\text{odd}} = -\sum\limits_{lmn} R_{il} R_{jm} R_{kn} \chi_{lmn}^{\text{odd}}. \end{cases} \tag{S11}$$

The constraint of χ_{ijk}^{odd} under grey MPG M_0 is equivalent to the isomorphic group $G_1 = G_0 \otimes \bar{1}$, leading to the vanishing of χ_{ijk}^{odd}. Because R and R' have the same symmetry constraint on χ_{ijk}^{even}, the transformation of χ_{ijk}^{even} under MPG M_0 equals to PG G_0. χ_{ijk}^{even} survives as long as grey MPG M_0 has no inversion symmetry. 20 of 32 grey MPGs without inversion symmetry have non-zero tensor elements, and their tensors are shown in Table IV of Supplementary Note 3.

For black-white (BW) MPGs $M_0 = G_0 + T(G_0 - S_0) = S_0 + R'S_0$. There are one-half unitary symmetry operations constituted by invariant subgroup S_0, and one-half of anti-unitary symmetry operations $R'S_0$ in BW MPGs. Because the constraint of R' on the χ_{ijk}^{even} acts as R, the symmetry of χ_{ijk}^{even} under BW MPG M_0 equals to χ_{ijk}^{even} under nonmagnetic PG of G_0 ($G_0 = S_0 + RS_0$). However, the constraint of anti-unitary operation R' on χ_{ijk}^{odd} is equivalent to a unitary operation IR ($I = \bar{1}$: inversion symmetry). Therefore, the transformation of χ_{ijk}^{odd} under the BW MPG M_0 is equivalent to a nonmagnetic PG G_1 with

$$G_1 = S_0 + I\,(RS_0) = S_0 + (IR)\,S_0. \tag{S12}$$

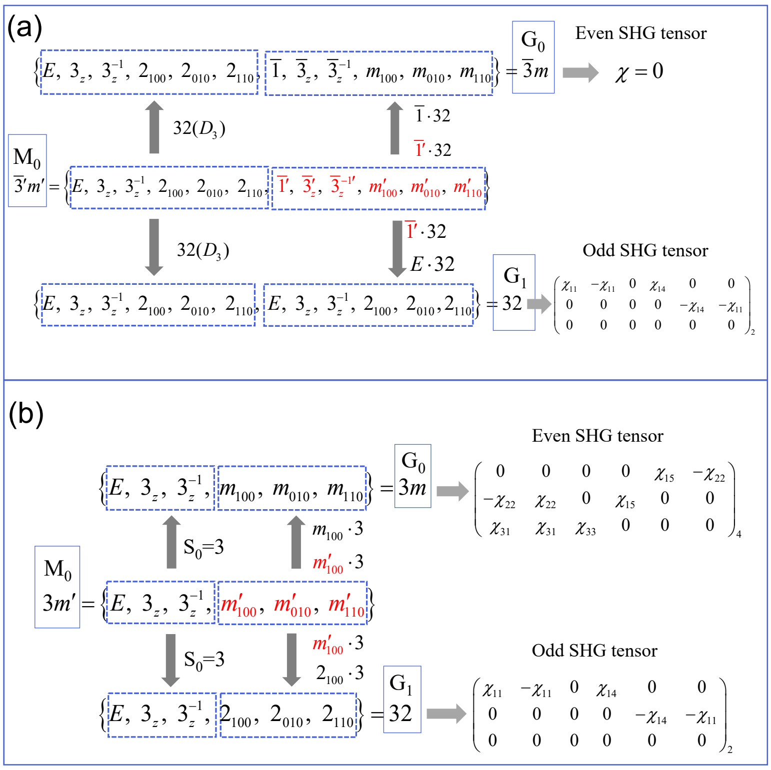
In other words, we simplify the symmetry of SHG in MPGs into non-magnetic PGs. Just looking for the SHG tensor under G_1 in Table IV in Supplementary Note 3, we could get the symmetries of χ_{ijk}^{even} and χ_{ijk}^{odd} under BW MPG M_0. According to Eq. (S12), the total 58 BW MPGs can be further divided into two subcases.

(3) BW MPGs M_0 have PT symmetry. In this case, $M_0 = S_0 + \bar{1}'S_0$, and G_0 has inversion symmetry. The even part of SHG vanishes, because PT symmetry ($\bar{1}'$) acts as the inversion symmetry for χ_{ijk}^{even}. According to Eq. (S12), G_1 becomes

$$G_1 = S_0 + (I \cdot I)\,S_0 = S_0, \ \textit{if}\ \bar{1}' \in R'S_0, \tag{S13}$$

i.e., G_1=S_0. The anti-unitary operations $\bar{1}'S_0$ have symmetry restriction on χ_{ijk}^{odd} as the unitary subgroup S_0. Therefore, the constraints of χ_{ijk}^{odd} under MPGs M_0 with PT operation are equivalent to the invariant subgroup S_0. An example of this type of MPG with $\bar{3}'m'$ is shown in Figure 1(a).

(4) BW MPGs M_0 have neither P ($\bar{1}$) nor PT ($\bar{1}'$) symmetry. In this case, the constraints of χ_{ijk}^{even} and χ_{ijk}^{odd} under M_0 are equivalent to nonmagnetic PGs G_0 and G_1, respectively. Besides, $G_1 \neq G_0$ (because $\bar{1} \notin S_0$)



Supplementary Figure 1: Two BW MPG examples. (a) $\bar{3}'m'$ and (b) $3m'$ to determine the even and odd SHG tensors. The SHG tensors here are used with the contracted notation, whose definition is in Eq. (S21).

and $G_1 \neq S_0$ (because $\bar{1}' \notin R'S_0$), i.e. G_1 and G_0 are the isomorphic groups as well. Instead of numerical calculation, just looking for the SHG tensor under G_0 and G_1 in Table IV in Supplementary Note 3, we will get the symmetries of χ_{ijk}^{even} and χ_{ijk}^{odd} respectively. An example of $3m'$ is shown in Figure 1(b), and the SHG symmetries of all BW MPGs are given in Table V of Supplementary Note 3. Because χ_{ijk}^{even} and χ_{ijk}^{odd} coexist and obey different symmetries, the total SHG tensor can be written as

$$\boldsymbol{\chi}^{(2)}(M_0) = \boldsymbol{\chi}^{\text{even}}(G_0) + \boldsymbol{\chi}^{\text{odd}}(G_1) = \chi(S_0),\ if\ \bar{1} \notin G_0. \tag{S14}$$

The last term is true because $G_0 \cap G_1 = S_0$.

For BW MPGs in Case 4, we find a very distinct phenomenon that the nonzero $\chi_{ijk}^{\text{odd}}$and χ_{ijk}^{even} tensor elements are mutually exclusive in most cases, except for $4'$, $\bar{4}'$, $\bar{4}2m'$, and $4'22'$, i.e., the nonzero χ_{ijk}^{odd} and χ_{ijk}^{even} are in different positions in SHG tensor (see Table V in Supplementary Note 3). It is because the constraint of symmetry 2 (C_2) and m (IC_2) on SHG tensors are opposite if symmetries locate on the coordinate axis. The anti-unitary operation $2'$ (m') constraint on χ_{ijk}^{even} is equal to 2 (m) symmetry, while on χ_{ijk}^{odd} to m (2) symmetry, therefore they lead to the nonzero odd and even SHG tensor elements are mutually exclusive. MPGs $4'$ and $\bar{4}'$ have no in-plane $2'$ or m' symmetry, and in-plane $2'$ or m' symmetry of $\bar{4}2m'$ and $4'22'$ is not along the x or y coordinate axis. Therefore, this rule are not suitable for these four MPGs.

To summarize, the characteristics of SHG under MPGs are summarized in Table I of the main text, and the SHG tensors of all 122 MPGs are listed in Supplementary Note 3, where χ_{ijk}^{even} and χ_{ijk}^{odd} and corresponding constraint groups G_0 and G_1 are also listed. Within the isomorphic group method, we simplify the SHG symmetry under MPGs into non-magnetic PGs efficiently. This method is free from complicated numerical calculations, and captures SHG rules clearly which are difficult before [7–9]. The above results are also suitable for the BPVE (bulk photovoltaic effect) tensors, because the BPVE susceptibility σ_{abc} $[J_a(0) = \sum_{bc} \sigma_{abc} E_b(\omega) E_c(-\omega)]$ has a similar expression as that of SHG, and both share similar symmetry constraints.

Supplementary Note 2. SYMMETRY ANALYSIS FOR LINEAR MAGNETO-OPTIC EFFECT IN ALL MPGS

Method 1: In the linear regime, the light induces alternating current (AC) in materials,

$$j_i(\omega) = \sum_j \sigma_{ij}(\omega) E_j(\omega) \tag{S15}$$

where σ_{ij} is the photoconductivity tensor. The transformation of σ_{ij} under the unitary operation is

$$R : \sigma_{ij} = \sum_{mn} R_{im} R_{jn} \sigma_{mn}. \tag{S16}$$

The transformation of σ_{ij} under the anti-unitary operation is

$$R' : \sigma_{ij} = \sum_{mn} R_{im} R_{jn} \sigma_{nm}. \tag{S17}$$

Eq. (S17) satisfy the Onsager reciprocal relationship $1'\sigma_{ij} = \sigma_{ji}$. With the above relationships (Eqs. (S16) and (S17)), we can drive the optical conductivity of every MPG. The full results of every MPG are studied in Ref. [9], and are listed in Bilbao Crystallographic Server/MTENSOR.

Photoconductivity tensor $[\sigma_{ij}]_{3\times3}$ has 9 elements, and it can be divided into two parts: symmetry part ($\sigma^S_{ij} = \sigma^S_{ji}$) with 6 independent elements and asymmetry part ($\sigma^A_{ij} = -\sigma^A_{ji}$) with 3 independent elements. Accordingly, $[\sigma_{ij}]_{3\times3}$ in Eq. (S15) can be rewritten as

$$[\sigma_{ij}] = \begin{bmatrix} \sigma^S_{xx} & \sigma^S_{xy} & \sigma^S_{xz} \\ \sigma^S_{xy} & \sigma^S_{yy} & \sigma^S_{yz} \\ \sigma^S_{xz} & \sigma^S_{yz} & \sigma^S_{zz} \end{bmatrix} + \begin{bmatrix} 0 & \sigma^A_{xy} & -\sigma^A_{zx} \\ -\sigma^A_{xy} & 0 & \sigma^A_{yz} \\ \sigma^A_{zx} & -\sigma^A_{yz} & 0 \end{bmatrix} \tag{S18}$$

The symmetry part is even under the time-reversal symmetry, and cannot lead to the linear magneto-optic effect (LMO). The LMO effect originates from the asymmetry part of optical conductivity σ^A_{ij} (anomalous photoconductivity), which satisfies $\sigma^A_{ij} = -\sigma^A_{ji}$.

Method 2: The asymmetry part in Eq. (S18) has three independent elements, and it is odd under time-reversal symmetry, which can be viewed as a pseudo-vector (axial tensor) $\mathbf{M} = (m_x, m_y, m_z)$, where $m_x \leftrightarrow \sigma^A_{yz}$, $m_y \leftrightarrow \sigma^A_{zx}$, $m_z \leftrightarrow \sigma^A_{xy}$. According to the transformation rules of pseudo-vector, R and IR have the same symmetry constrain on $\mathbf{M}$:

$$IR\mathbf{M} = R\mathbf{M}. \tag{S19}$$

The improper rotation operation (IR) act as a proper rotation operation (R) for pseudo-vector, and this leads to the original point group of C_{nv} ($2mm$, $3m$, $4mm$, $6mm$), D_n (222, 32, 422, 622), D_{nh} (mmm, $\bar{6}m2$, $4/mmm$, $6/mmm$), D_{nd} ($\bar{3}m$, $\bar{4}m2$) and cubic point groups T (23), O (432), T_d ($\bar{4}3m$), T_h ($m\bar{3}$), O_h ($m\bar{3}m$) zero.

For the anti-unitary operation,

$$R'\mathbf{M} = -R\mathbf{M}, \tag{S20}$$

because T operation reverses $\mathbf{M}$. According to Eq. (S20), the pseudo-vector is zero for grey MPGs and black-white MPGs with PT ($G' = S + IS'$) symmetry. Besides, the anti-unitary operation R' ($R \geq 3$) also leads to the vanishing of the pseudo-vector $\mathbf{M}$.

Based on the above analysis, there are 31 MPGs (13 original MPGs and 18 black-white MPGs) have the nonzero asymmetry part of photoconductivity (i.e., linear magneto-optic effect), which are listed in Table II. The results are consistent with that Refs. [13–15].

Suppl. Tab. II: MPG with linear magneto-optic effect, and corresponding asymmetry part and asymmetry part of photoconductivity.

Crystallographic system	**MPG**	**Axial vector M**	**Asymmetry part**	**Symmetry part**
Triclinic	1, $\bar{1}$	(m_x, m_y, m_z)	$\begin{bmatrix} 0 & \sigma_{xy} & -\sigma_{zx} \\ -\sigma_{xy} & 0 & \sigma_{yz} \\ \sigma_{zx} & -\sigma_{yz} & 0 \end{bmatrix}_3$	$\begin{bmatrix} \sigma_{xx} & \sigma_{xy} & \sigma_{xz} \\ \sigma_{xy} & \sigma_{yy} & \sigma_{yz} \\ \sigma_{xz} & \sigma_{yz} & \sigma_{zz} \end{bmatrix}_6$
Monoclinic	Original point group: 2, $2/m$ ($2//y$), m ($m \perp y$)	$(0, m_y, 0)$	$\begin{bmatrix} 0 & 0 & -\sigma_{zx} \\ 0 & 0 & 0 \\ \sigma_{zx} & 0 & 0 \end{bmatrix}_1$	$\begin{bmatrix} \sigma_{xx} & 0 & \sigma_{xz} \\ 0 & \sigma_{yy} & 0 \\ \sigma_{xz} & 0 & \sigma_{zz} \end{bmatrix}_4$
	Black-White group: $2'$, m', $2'/m'$	$(m_x, 0, m_z)$	$\begin{bmatrix} 0 & \sigma_{xy} & 0 \\ -\sigma_{xy} & 0 & \sigma_{yz} \\ 0 & -\sigma_{yz} & 0 \end{bmatrix}_2$	
Orthorhombic	Black-White group: $2'2'2$, $m'm'2$, $m'm'm$	$(0, 0, m_z)$	$\begin{bmatrix} 0 & \sigma_{xy} & 0 \\ -\sigma_{xy} & 0 & 0 \\ 0 & 0 & 0 \end{bmatrix}_1$	$\begin{bmatrix} \sigma_{xx} & 0 & 0 \\ 0 & \sigma_{yy} & 0 \\ 0 & 0 & \sigma_{zz} \end{bmatrix}_3$
	Black-White group: $m'm2'$	$(0, m_y, 0)$	$\begin{bmatrix} 0 & 0 & -\sigma_{zx} \\ 0 & 0 & 0 \\ \sigma_{zx} & 0 & 0 \end{bmatrix}_1$	
Tetragonal, Trigonal, Hexagonal	Original point group: 4, $\bar{4}$, $4/m$, 3, $\bar{3}$, 6, $\bar{6}$, $6/m$	$(0, 0, m_z)$	$\begin{bmatrix} 0 & \sigma_{xy} & 0 \\ -\sigma_{xy} & 0 & 0 \\ 0 & 0 & 0 \end{bmatrix}_1$	$\begin{bmatrix} \sigma_{xx} & 0 & 0 \\ 0 & \sigma_{xx} & 0 \\ 0 & 0 & \sigma_{zz} \end{bmatrix}_2$
	Black-White group: $42'2'$, $4m'm'$, $\bar{4}2'm'$, $4/mm'm'$, $32'$, $3m'$, $\bar{3}m'$, $62'2'$, $6m'm'$, $\bar{6}m'2'$, $6/mm'm'$			

Supplementary Note 3. SHG AND LMO EFFECT SYMMETRY DICTIONARY IN ALL MPGS

Suppl. Note 3.1. Lattice character directions of crystallographic systems

Since the symmetries of the tensors depend on the choice of the coordinate system, we introduce lattice character directions of crystallographic systems adopted in our work. One can also refer *International Tables for Crystallography - Vol. A* [16] for details.

Suppl. Tab. III: Lattice character directions of 32 original point groups.

Crystallographic system	**Point Groups**	**Direction 1**	**Direction 2**	**Direction 3**
Cubic	23, $m\bar{3}$, 432, $\bar{4}3m$, $m\bar{3}m$	$\mathbf{a}/\mathbf{b}/\mathbf{c}$	body diagonal *e.g.* $\mathbf{a}+\mathbf{b}+\mathbf{c}$	face diagonal *e.g.* $\mathbf{a}+\mathbf{b}$
Hexagonal	6, $\bar{6}$, $6/m$, 622, $6mm$, $\bar{6}m2$, $6/mmm$	$\mathbf{c}$	$\mathbf{a}/\mathbf{b}$	$\mathbf{a}+\mathbf{2b}/\mathbf{2a}+\mathbf{b}$
Tetragonal	4, $\bar{4}$, $4/m$, 422, $4mm$, $\bar{4}2m$, $4/mmm$	$\mathbf{c}$	$\mathbf{a}/\mathbf{b}$	face diagonal *e.g.* $\mathbf{a}+\mathbf{b}$
Trigonal	3, $\bar{3}$, 32, $3m$, $\bar{3}m$	$\mathbf{c}$	$\mathbf{a}/\mathbf{b}$	NA
Orthorhombic	222, $mm2$, mmm	$\mathbf{a}$	$\mathbf{b}$	$\mathbf{c}$
Monoclinic	2, m, $2/m$	$\mathbf{b}$ (unique axis *b*)	NA	NA
Triclinic	1, $\bar{1}$	NA	NA	NA

1. 'NA' (not available) in the third to the fifth column denotes no symmetries along these character directions.
2. '/' in the third to the fifth column denotes there are two or more equivalent character directions.
3. The character directions for grey MPGs and black-white MPGs obey similar rules to original MPGs.

Suppl. Note 3.2. SHG tensor notation

Because the SHG elements $\chi^{(2)}_{ijk}$ have the subscripts-switch symmetry, i.e., $\chi^{(2)}_{ijk} = \chi^{(2)}_{ikj}$, the $[\chi^{(2)}_{ijk}]_{3\times3\times3}$ tensor can be contracted as a 3×6 matrix $\left[\chi^{(2)}_{il}\right]_{3\times6}$ using the following simplified indices [11, 12]:

$$\begin{array}{ccccccc} jk \rightarrow & 11 & 22 & 33 & 23,32 & 31,13 & 21,12 \\ l \rightarrow & 1 & 2 & 3 & 4 & 5 & 6 \end{array} \tag{S21}$$

With the above notation, the nonlinear response can be rewritten as

$$\begin{pmatrix} P_1(2\omega) \\ P_2(2\omega) \\ P_3(2\omega) \end{pmatrix} = \begin{pmatrix} \chi_{11} & \chi_{12} & \chi_{13} & \chi_{14} & \chi_{15} & \chi_{16} \\ \chi_{21} & \chi_{22} & \chi_{23} & \chi_{24} & \chi_{25} & \chi_{26} \\ \chi_{31} & \chi_{32} & \chi_{33} & \chi_{34} & \chi_{35} & \chi_{36} \end{pmatrix} \begin{pmatrix} E_1^2(\omega) \\ E_2^2(\omega) \\ E_3^2(\omega) \\ 2E_2(\omega)E_3(\omega) \\ 2E_1(\omega)E_3(\omega) \\ 2E_1(\omega)E_2(\omega) \end{pmatrix}. \tag{S22}$$

In the following, the SHG tensors are adopted the form with 3×6 matrices, as shown in Eq. (S22).

Suppl. Note 3.3. Symmetry of SHG and LMO effect tables in 32 grey and 32 original MPGs

Suppl. Tab. IV: SHG and LMO symmetries of 32 grey and 32 original MPGs. Note: (1) The meanings of i and l in 3×6 SHG tensor χ_{il} refer to Eq. (S21) and Eq. (S22). (2) The subscript number of each SHG tensor represents the independent element number. (3) There is only the even part (χ_{il}^{even}) for grey MPGs (with $1'$), and the odd (χ_{il}^{odd}) and even (χ_{il}^{even}) parts and have same symmetry in original MPGs (the first one of each row, without $1'$). (4) The symmetries of LMO are presented in Table II of Supplementary Note 2. (5)The following table can also be found in the home-made website "Classification of SHG effect in magnetic materials".

MPG	SHG tensor $[\chi_{il}^{(2)}]_{3\times 6}$	LMO effect of original MPG
1 (1.1.1) $11'$ (1.2.2)	$\begin{pmatrix} \chi_{11} & \chi_{12} & \chi_{13} & \chi_{14} & \chi_{15} & \chi_{16} \\ \chi_{21} & \chi_{22} & \chi_{23} & \chi_{24} & \chi_{25} & \chi_{26} \\ \chi_{31} & \chi_{32} & \chi_{33} & \chi_{34} & \chi_{35} & \chi_{36} \end{pmatrix}_{18}$	✓
$\bar{1}$ (2.1.3) $\bar{1}1'$ (2.2.4)	χ=0	✓
2 (3.1.6) $21'$ (3.2.7)	$\begin{pmatrix} 0 & 0 & 0 & \chi_{14} & 0 & \chi_{16} \\ \chi_{21} & \chi_{22} & \chi_{23} & 0 & \chi_{25} & 0 \\ 0 & 0 & 0 & \chi_{34} & 0 & \chi_{36} \end{pmatrix}_{8}$	✓
m (4.1.9) $m1'$ (4.2.10)	$\begin{pmatrix} \chi_{11} & \chi_{12} & \chi_{13} & 0 & \chi_{15} & 0 \\ 0 & 0 & 0 & \chi_{24} & 0 & \chi_{26} \\ \chi_{31} & \chi_{32} & \chi_{33} & 0 & \chi_{35} & 0 \end{pmatrix}_{10}$	✓
$2/m$ (5.1.12) $2/m1'$ (5.2.13)	χ=0	✓
222 (6.1.17) $2221'$ (6.2.18)	$\begin{pmatrix} 0 & 0 & 0 & \chi_{14} & 0 & 0 \\ 0 & 0 & 0 & 0 & \chi_{25} & 0 \\ 0 & 0 & 0 & 0 & 0 & \chi_{36} \end{pmatrix}_{3}$	×
$mm2$ (7.1.20) $mm21'$ (7.2.21)	$\begin{pmatrix} 0 & 0 & 0 & 0 & \chi_{15} & 0 \\ 0 & 0 & 0 & \chi_{24} & 0 & 0 \\ \chi_{31} & \chi_{32} & \chi_{33} & 0 & 0 & 0 \end{pmatrix}_{5}$	×
mmm (8.1.24) $mmm1'$ (8.2.25)	χ=0	×
4 (9.1.29) $41'$ (9.2.30)	$\begin{pmatrix} 0 & 0 & 0 & \chi_{14} & \chi_{15} & 0 \\ 0 & 0 & 0 & \chi_{15} & -\chi_{14} & 0 \\ \chi_{31} & \chi_{31} & \chi_{33} & 0 & 0 & 0 \end{pmatrix}_{4}$	✓
$\bar{4}$ (10.1.32) $\bar{4}1'$ (10.2.33)	$\begin{pmatrix} 0 & 0 & 0 & \chi_{14} & \chi_{15} & 0 \\ 0 & 0 & 0 & -\chi_{15} & \chi_{14} & 0 \\ \chi_{33} & -\chi_{31} & 0 & 0 & 0 & \chi_{36} \end{pmatrix}_{4}$	✓
$4/m$ (11.1.35) $4/m1'$ (11.2.36)	χ=0	✓
422 (12.1.40) $4221'$ (12.2.41)	$\begin{pmatrix} 0 & 0 & 0 & \chi_{14} & 0 & 0 \\ 0 & 0 & 0 & 0 & -\chi_{14} & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 \end{pmatrix}_{1}$	×

Continued on next page

Suppl. Tab. IV – continued from previous page

MPG	SHG tensor $[\chi^{(2)}_{il}]_{3\times 6}$	LMO effect of original MPG
$4mm$ (13.1.44) $4mm1'$ (13.2.45)	$\begin{pmatrix} 0 & 0 & 0 & 0 & \chi_{15} & 0 \\ 0 & 0 & 0 & \chi_{15} & 0 & 0 \\ \chi_{31} & \chi_{31} & \chi_{33} & 0 & 0 & 0 \end{pmatrix}_3$	×
$\bar{4}2m$ (14.1.48) $\bar{4}2m1'$ (14.2.49)	$\begin{pmatrix} 0 & 0 & 0 & \chi_{14} & 0 & 0 \\ 0 & 0 & 0 & 0 & \chi_{14} & 0 \\ 0 & 0 & 0 & 0 & 0 & \chi_{36} \end{pmatrix}_2$	×
$4/mmm$ (15.1.53) $4/mmm1'$ (15.2.54)	χ=0	×
3 (16.1.60) $31'$ (16.2.61)	$\begin{pmatrix} \chi_{11} & -\chi_{11} & 0 & \chi_{14} & \chi_{15} & -\chi_{22} \\ -\chi_{22} & \chi_{22} & 0 & \chi_{15} & -\chi_{14} & -\chi_{11} \\ \chi_{31} & \chi_{31} & \chi_{33} & 0 & 0 & 0 \end{pmatrix}_6$	✓
$\bar{3}$ (17.1.62) $\bar{3}1'$ (17.2.63)	χ=0	✓
32 (18.1.65) $321'$ (18.2.66)	$\begin{pmatrix} \chi_{11} & -\chi_{11} & 0 & \chi_{14} & 0 & 0 \\ 0 & 0 & 0 & 0 & -\chi_{14} & -\chi_{11} \\ 0 & 0 & 0 & 0 & 0 & 0 \end{pmatrix}_2$	×
$3m$ (19.1.68) $3m1'$ (19.2.69)	$\begin{pmatrix} 0 & 0 & 0 & 0 & \chi_{15} & -\chi_{22} \\ -\chi_{22} & \chi_{22} & 0 & \chi_{15} & 0 & 0 \\ \chi_{31} & \chi_{31} & \chi_{33} & 0 & 0 & 0 \end{pmatrix}_4$	×
$\bar{3}m$ (20.1.71) $\bar{3}m1'$ (20.2.72)	χ=0	×
6 (21.1.76) $61'$ (21.2.77)	$\begin{pmatrix} 0 & 0 & 0 & \chi_{14} & \chi_{15} & 0 \\ 0 & 0 & 0 & \chi_{15} & -\chi_{14} & 0 \\ \chi_{31} & \chi_{31} & \chi_{33} & 0 & 0 & 0 \end{pmatrix}_4$	✓
$\bar{6}$ (22.1.79) $\bar{6}1'$ (22.2.80)	$\begin{pmatrix} \chi_{11} & -\chi_{11} & 0 & 0 & 0 & -\chi_{22} \\ -\chi_{22} & \chi_{22} & 0 & 0 & 0 & -\chi_{11} \\ 0 & 0 & 0 & 0 & 0 & 0 \end{pmatrix}_2$	✓
$6/m$ (23.1.82) $6/m1'$ (23.2.83)	χ=0	✓
622 (24.1.87) $6221'$ (24.2.88)	$\begin{pmatrix} 0 & 0 & 0 & \chi_{14} & 0 & 0 \\ 0 & 0 & 0 & 0 & -\chi_{14} & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 \end{pmatrix}_1$	×
$6mm$ (25.1.91) $6mm1'$ (25.2.92)	$\begin{pmatrix} 0 & 0 & 0 & 0 & \chi_{15} & 0 \\ 0 & 0 & 0 & \chi_{15} & 0 & 0 \\ \chi_{31} & \chi_{31} & \chi_{33} & 0 & 0 & 0 \end{pmatrix}_3$	×
$\bar{6}m2$ (26.1.95) $\bar{6}m21'$ (26.2.96)	$\begin{pmatrix} 0 & 0 & 0 & 0 & 0 & -\chi_{22} \\ -\chi_{22} & \chi_{22} & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 \end{pmatrix}_1$	×
$6/mmm$ (27.1.100) $6/mmm1'$ (27.2.101)	χ=0	×

Continued on next page

Suppl. Tab. IV – continued from previous page

MPG	SHG tensor $[\chi^{(2)}_{il}]_{3\times6}$	LMO effect of original MPG
23 (28.1.107) $231'$ (28.2.108)	$\begin{pmatrix} 0 & 0 & 0 & \chi_{14} & 0 & 0 \\ 0 & 0 & 0 & 0 & \chi_{14} & 0 \\ 0 & 0 & 0 & 0 & 0 & \chi_{14} \end{pmatrix}_1$	×
$m\bar{3}$ (29.1.109) $m\bar{3}1'$ (29.2.110)	χ=0	×
432 (30.1.112) $4321'$ (30.2.113)	χ=0	×
$\bar{4}3m$ (31.1.115) $\bar{4}3m1'$ (31.2.116)	$\begin{pmatrix} 0 & 0 & 0 & \chi_{14} & 0 & 0 \\ 0 & 0 & 0 & 0 & \chi_{14} & 0 \\ 0 & 0 & 0 & 0 & 0 & \chi_{14} \end{pmatrix}_1$	×
$m\bar{3}m$ (32.1.118) $m\bar{3}m1'$ (32.2.119)	χ=0	×

Suppl. Note 3.4. Symmetry of SHG and LMO effect tables in 58 BW MPGs

Suppl. Tab. V: SHG and LMO symmetries of 58 BW MPGs. Note: (1) MPG $M_0 = S_0 + T(G_0 - S_0) = S_0 + R'S_0$. (2) The subscript number of the SHG tensor means the independent element number. (3) The symmetries of the LMO effect refer to Table II of Supplementary Note 2. (4)The following table can also be found in the home-made website "Classification of SHG effect in magnetic materials".

MPG M_0	PG G_0	S_0	R'	G_0 and $[\chi^{\text{even}}_{il}]_{3\times6}$	G_1 and $[\chi^{\text{odd}}_{il}]_{3\times6}$	LMO
$\bar{1}'$ (2.3.5)	$\bar{1}$	1	$\bar{1}'$	$\bar{1}$ χ=0	1 $\begin{pmatrix} \chi_{11} & \chi_{12} & \chi_{13} & \chi_{14} & \chi_{15} & \chi_{16} \\ \chi_{21} & \chi_{22} & \chi_{23} & \chi_{24} & \chi_{25} & \chi_{26} \\ \chi_{31} & \chi_{32} & \chi_{33} & \chi_{34} & \chi_{35} & \chi_{36} \end{pmatrix}_{18}$	×
$2'$ $(2//y)$ (3.3.8)	2	1	$2'_{010}$	2 $\begin{pmatrix} 0 & 0 & 0 & \chi_{14} & 0 & \chi_{16} \\ \chi_{21} & \chi_{22} & \chi_{23} & 0 & \chi_{25} & 0 \\ 0 & 0 & 0 & \chi_{34} & 0 & \chi_{36} \end{pmatrix}_8$	m $\begin{pmatrix} \chi_{11} & \chi_{12} & \chi_{13} & 0 & \chi_{15} & 0 \\ 0 & 0 & 0 & \chi_{24} & 0 & \chi_{26} \\ \chi_{31} & \chi_{32} & \chi_{33} & 0 & \chi_{35} & 0 \end{pmatrix}_{10}$	✓
m' $(m \perp y)$ (4.3.11)	m	1	m'_{010}	m $\begin{pmatrix} \chi_{11} & \chi_{12} & \chi_{13} & 0 & \chi_{15} & 0 \\ 0 & 0 & 0 & \chi_{24} & 0 & \chi_{26} \\ \chi_{31} & \chi_{32} & \chi_{33} & 0 & \chi_{35} & 0 \end{pmatrix}_{10}$	2 $\begin{pmatrix} 0 & 0 & 0 & \chi_{14} & 0 & \chi_{16} \\ \chi_{21} & \chi_{22} & \chi_{23} & 0 & \chi_{25} & 0 \\ 0 & 0 & 0 & \chi_{34} & 0 & \chi_{36} \end{pmatrix}_8$	✓
$2'/m$ $(2//y)$ (5.3.14)	$2/m$	m	$\bar{1}'$	$2/m$ χ=0	m $\begin{pmatrix} \chi_{11} & \chi_{12} & \chi_{13} & 0 & \chi_{15} & 0 \\ 0 & 0 & 0 & \chi_{24} & 0 & \chi_{26} \\ \chi_{31} & \chi_{32} & \chi_{33} & 0 & \chi_{35} & 0 \end{pmatrix}_{10}$	×

Continued on next page

Suppl. Tab. V – continued from previous page

MPG M_0	**PG** G_0	S_0	R'	G_0 and $[\chi^{\rm even}_{il}]_{3\times6}$	G_1 and $[\chi^{\rm odd}_{il}]_{3\times6}$	**LMC**
$2/m'$ $(2//y)$ (5.4.15)	$2/m$	2	$\bar{1}'$	$2/m$ χ=0	2 $\begin{pmatrix} 0 & 0 & 0 & \chi_{14} & 0 & \chi_{16} \\ \chi_{21} & \chi_{22} & \chi_{23} & 0 & \chi_{25} & 0 \\ 0 & 0 & 0 & \chi_{34} & 0 & \chi_{36} \end{pmatrix}_8$	$\times$
$2'/m'$ $(2//y)$ (5.5.16)	$2/m$	$\bar{1}$	$2'$	$2/m$ χ=0	$2/m$ χ=0	✓
$2'2'2$ (6.3.19)	222	2 $(2//z)$	$2'_{100}$	222 $\begin{pmatrix} 0 & 0 & 0 & \chi_{14} & 0 & 0 \\ 0 & 0 & 0 & 0 & \chi_{25} & 0 \\ 0 & 0 & 0 & 0 & 0 & \chi_{36} \end{pmatrix}_3$	$mm2$ $\begin{pmatrix} 0 & 0 & 0 & 0 & \chi_{15} & 0 \\ 0 & 0 & 0 & \chi_{24} & 0 & 0 \\ \chi_{31} & \chi_{32} & \chi_{33} & 0 & 0 & 0 \end{pmatrix}_5$	✓
$m'm2'$ $(2//z)$ (7.3.22)	$mm2$	m $(m\perp y)$	$2'_{001}$	$mm2$ $\begin{pmatrix} 0 & 0 & 0 & 0 & \chi_{15} & 0 \\ 0 & 0 & 0 & \chi_{24} & 0 & 0 \\ \chi_{31} & \chi_{32} & \chi_{33} & 0 & 0 & 0 \end{pmatrix}_5$	$2mm$ $\begin{pmatrix} \chi_{11} & \chi_{12} & \chi_{13} & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & \chi_{26} \\ 0 & 0 & 0 & 0 & \chi_{35} & 0 \end{pmatrix}_5$	✓
$m'm'2$ $(2//z)$ (7.4.23)	$mm2$	2 $(2//z)$	m'_{100}	$mm2$ $\begin{pmatrix} 0 & 0 & 0 & 0 & \chi_{15} & 0 \\ 0 & 0 & 0 & \chi_{24} & 0 & 0 \\ \chi_{31} & \chi_{32} & \chi_{33} & 0 & 0 & 0 \end{pmatrix}_5$	222 $\begin{pmatrix} 0 & 0 & 0 & \chi_{14} & 0 & 0 \\ 0 & 0 & 0 & 0 & \chi_{25} & 0 \\ 0 & 0 & 0 & 0 & 0 & \chi_{36} \end{pmatrix}_3$	✓
mmm' (8.3.26)	mmm	$mm2$	$\bar{1}'$	mmm χ=0	$mm2$ $\begin{pmatrix} 0 & 0 & 0 & 0 & \chi_{15} & 0 \\ 0 & 0 & 0 & \chi_{24} & 0 & 0 \\ \chi_{31} & \chi_{32} & \chi_{33} & 0 & 0 & 0 \end{pmatrix}_5$	$\times$
$m'm'm$ (8.4.27)	mmm	$2/m$ $(2//z)$	m'_{100}	mmm χ=0	mmm χ=0	✓
$m'm'm'$ (8.5.28)	mmm	222	$\bar{1}'$	mmm χ=0	222 $\begin{pmatrix} 0 & 0 & 0 & \chi_{14} & 0 & 0 \\ 0 & 0 & 0 & 0 & \chi_{25} & 0 \\ 0 & 0 & 0 & 0 & 0 & \chi_{36} \end{pmatrix}_3$	$\times$
$4'$ (9.3.31)	4	2 $(2//z)$	$4'_{001}$	4 $\begin{pmatrix} 0 & 0 & 0 & \chi_{14} & \chi_{15} & 0 \\ 0 & 0 & 0 & \chi_{15} & -\chi_{14} & 0 \\ \chi_{31} & \chi_{31} & \chi_{33} & 0 & 0 & 0 \end{pmatrix}_4$	$\bar{4}$ $\begin{pmatrix} 0 & 0 & 0 & \chi_{14} & \chi_{15} & 0 \\ 0 & 0 & 0 & -\chi_{15} & \chi_{14} & 0 \\ \chi_{33} & -\chi_{31} & 0 & 0 & 0 & \chi_{36} \end{pmatrix}_4$	$\times$
$\bar{4}'$ (10.3.34)	$\bar{4}$	2 $(2//z)$	$\bar{4}'_{001}$	$\bar{4}$ $\begin{pmatrix} 0 & 0 & 0 & \chi_{14} & \chi_{15} & 0 \\ 0 & 0 & 0 & -\chi_{15} & \chi_{14} & 0 \\ \chi_{33} & -\chi_{31} & 0 & 0 & 0 & \chi_{36} \end{pmatrix}_4$	4 $\begin{pmatrix} 0 & 0 & 0 & \chi_{14} & \chi_{15} & 0 \\ 0 & 0 & 0 & \chi_{15} & -\chi_{14} & 0 \\ \chi_{31} & \chi_{31} & \chi_{33} & 0 & 0 & 0 \end{pmatrix}_4$	$\times$
$4'/m$ (11.3.37)	$4/m$	$2/m$	$4'_{001}$	$4/m$ χ=0	$4/m$ χ=0	$\times$

Continued on next page

Suppl. Tab. V – continued from previous page

MPG M_0	**PG** G_0	S_0	R'	G_0 and $[\chi_{il}^{\text{even}}]_{3\times 6}$	G_1 and $[\chi_{il}^{\text{odd}}]_{3\times 6}$	**LMC**
$4/m'$ (11.4.38)	$4/m$	4	$\bar{1}'$	$4/m$ χ=0	4 $\begin{pmatrix} 0 & 0 & 0 & \chi_{14} & \chi_{15} & 0 \\ 0 & 0 & 0 & \chi_{15} & -\chi_{14} & 0 \\ \chi_{31} & \chi_{31} & \chi_{33} & 0 & 0 & 0 \end{pmatrix}_4$	×
$4'/m'$ (11.5.39)	$4/m$	$\bar{4}$	$\bar{1}'$	$4/m$ χ=0	$\bar{4}$ $\begin{pmatrix} 0 & 0 & 0 & \chi_{14} & \chi_{15} & 0 \\ 0 & 0 & 0 & -\chi_{15} & \chi_{14} & 0 \\ \chi_{33} & -\chi_{31} & 0 & 0 & 0 & \chi_{36} \end{pmatrix}_4$	×
$4'22'$ (12.3.42)	422	222	$4'_{001}$	422 $\begin{pmatrix} 0 & 0 & 0 & \chi_{14} & 0 & 0 \\ 0 & 0 & 0 & 0 & -\chi_{14} & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 \end{pmatrix}_1$	$\bar{4}2m$ $\begin{pmatrix} 0 & 0 & 0 & \chi_{14} & 0 & 0 \\ 0 & 0 & 0 & 0 & \chi_{14} & 0 \\ 0 & 0 & 0 & 0 & 0 & \chi_{36} \end{pmatrix}_2$	×
$42'2'$ (12.4.43)	422	4	$2'_{100}$	422 $\begin{pmatrix} 0 & 0 & 0 & \chi_{14} & 0 & 0 \\ 0 & 0 & 0 & 0 & -\chi_{14} & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 \end{pmatrix}_1$	$4mm$ $\begin{pmatrix} 0 & 0 & 0 & 0 & \chi_{15} & 0 \\ 0 & 0 & 0 & \chi_{15} & 0 & 0 \\ \chi_{31} & \chi_{31} & \chi_{33} & 0 & 0 & 0 \end{pmatrix}_3$	✓
$4'm'm$ (13.3.46)	$4mm$	$2mm$	$4'_{001}$	$4mm$ $\begin{pmatrix} 0 & 0 & 0 & 0 & \chi_{15} & 0 \\ 0 & 0 & 0 & \chi_{15} & 0 & 0 \\ \chi_{31} & \chi_{31} & \chi_{33} & 0 & 0 & 0 \end{pmatrix}_3$	$\bar{4}2m$ $\begin{pmatrix} 0 & 0 & 0 & \chi_{14} & 0 & 0 \\ 0 & 0 & 0 & 0 & \chi_{14} & 0 \\ 0 & 0 & 0 & 0 & 0 & \chi_{36} \end{pmatrix}_2$	×
$4m'm'$ (13.4.47)	$4mm$	4	m'_{100}	$4mm$ $\begin{pmatrix} 0 & 0 & 0 & 0 & \chi_{15} & 0 \\ 0 & 0 & 0 & \chi_{15} & 0 & 0 \\ \chi_{31} & \chi_{31} & \chi_{33} & 0 & 0 & 0 \end{pmatrix}_3$	422 $\begin{pmatrix} 0 & 0 & 0 & \chi_{14} & 0 & 0 \\ 0 & 0 & 0 & 0 & -\chi_{14} & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 \end{pmatrix}_1$	✓
$\bar{4}'2'm$ (14.3.50)	$\bar{4}2m$	$2mm$	$\bar{4}'$	$\bar{4}2m$ $\begin{pmatrix} 0 & 0 & 0 & \chi_{14} & 0 & 0 \\ 0 & 0 & 0 & 0 & \chi_{14} & 0 \\ 0 & 0 & 0 & 0 & 0 & \chi_{36} \end{pmatrix}_2$	$4mm$ $\begin{pmatrix} 0 & 0 & 0 & 0 & \chi_{15} & 0 \\ 0 & 0 & 0 & \chi_{15} & 0 & 0 \\ \chi_{31} & \chi_{31} & \chi_{33} & 0 & 0 & 0 \end{pmatrix}_3$	×
$\bar{4}'2m'$ (14.4.51)	$\bar{4}2m$	222	$\bar{4}'$	$\bar{4}2m$ $\begin{pmatrix} 0 & 0 & 0 & \chi_{14} & 0 & 0 \\ 0 & 0 & 0 & 0 & \chi_{14} & 0 \\ 0 & 0 & 0 & 0 & 0 & \chi_{36} \end{pmatrix}_2$	422 $\begin{pmatrix} 0 & 0 & 0 & \chi_{14} & 0 & 0 \\ 0 & 0 & 0 & 0 & -\chi_{14} & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 \end{pmatrix}_1$	×
$\bar{4}2'm'$ (14.5.52)	$\bar{4}2m$	$\bar{4}$	$2'_{100}$	$\bar{4}2m$ $\begin{pmatrix} 0 & 0 & 0 & \chi_{14} & 0 & 0 \\ 0 & 0 & 0 & 0 & \chi_{14} & 0 \\ 0 & 0 & 0 & 0 & 0 & \chi_{36} \end{pmatrix}_2$	$\bar{4}m2$ $\begin{pmatrix} 0 & 0 & 0 & 0 & \chi_{15} & 0 \\ 0 & 0 & 0 & -\chi_{15} & 0 & 0 \\ \chi_{31} & -\chi_{31} & 0 & 0 & 0 & 0 \end{pmatrix}_2$	✓
$4/m'mm$ (15.3.55)	$4/mmm$	$4mm$	$\bar{1}'$	$4/mmm$ χ=0	$4mm$ $\begin{pmatrix} 0 & 0 & 0 & 0 & \chi_{15} & 0 \\ 0 & 0 & 0 & \chi_{15} & 0 & 0 \\ \chi_{31} & \chi_{31} & \chi_{33} & 0 & 0 & 0 \end{pmatrix}_3$	×

Continued on next page

Suppl. Tab. V – continued from previous page

MPG M_0	PG G_0	S_0	R'	G_0 and $[\chi_{il}^{\text{even}}]_{3\times6}$	G_1 and $[\chi_{il}^{\text{odd}}]_{3\times6}$	LMC
$4'/mm'm$ (15.4.56)	$4/mmm$	mmm	$\bar{4}'$	$4/mmm$ χ=0	$4/mmm$ χ=0	×
$4'/m'm'm$ (15.5.57)	$4/mmm$	$\bar{4}2m$	$\bar{1}'$	$4/mmm$ χ=0	$\bar{4}2m$ $\begin{pmatrix} 0 & 0 & 0 & \chi_{14} & 0 & 0 \\ 0 & 0 & 0 & 0 & \chi_{14} & 0 \\ 0 & 0 & 0 & 0 & 0 & \chi_{36} \end{pmatrix}_2$	×
$4/mm'm'$ (15.6.58)	$4/mmm$	$4/m$	$2'_{100}$	$4/mmm$ χ=0	$4/mmm$ χ=0	✓
$4/m'm'm'$ (15.7.59)	$4/mmm$	422	$\bar{1}'$	$4/mmm$ χ=0	422 $\begin{pmatrix} 0 & 0 & 0 & \chi_{14} & 0 & 0 \\ 0 & 0 & 0 & 0 & -\chi_{14} & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 \end{pmatrix}_1$	×
$\bar{3}'$ (17.3.64)	$\bar{3}$	3	$\bar{1}'$	$\bar{3}$ χ=0	3 $\begin{pmatrix} \chi_{11} & -\chi_{11} & 0 & \chi_{14} & \chi_{15} & -\chi_{22} \\ -\chi_{22} & \chi_{22} & 0 & \chi_{15} & -\chi_{14} & -\chi_{11} \\ \chi_{31} & \chi_{31} & \chi_{33} & 0 & 0 & 0 \end{pmatrix}$	×
$32'$ (18.3.67)	32	3	$2'_{100}$	32 $\begin{pmatrix} \chi_{11} & -\chi_{11} & 0 & \chi_{14} & 0 & 0 \\ 0 & 0 & 0 & 0 & -\chi_{14} & -\chi_{11} \\ 0 & 0 & 0 & 0 & 0 & 0 \end{pmatrix}_2$	$3m$ $\begin{pmatrix} 0 & 0 & 0 & 0 & \chi_{15} & -\chi_{22} \\ -\chi_{22} & \chi_{22} & 0 & \chi_{15} & 0 & 0 \\ \chi_{31} & \chi_{31} & \chi_{33} & 0 & 0 & 0 \end{pmatrix}_4$	✓
$3m'$ (19.3.70)	$3m$	3	m'_{100}	$3m$ $\begin{pmatrix} 0 & 0 & 0 & 0 & \chi_{15} & -\chi_{22} \\ -\chi_{22} & \chi_{22} & 0 & \chi_{15} & 0 & 0 \\ \chi_{31} & \chi_{31} & \chi_{33} & 0 & 0 & 0 \end{pmatrix}_4$	32 $\begin{pmatrix} \chi_{11} & -\chi_{11} & 0 & \chi_{14} & 0 & 0 \\ 0 & 0 & 0 & 0 & -\chi_{14} & -\chi_{11} \\ 0 & 0 & 0 & 0 & 0 & 0 \end{pmatrix}_2$	✓
$\bar{3}'m$ (20.3.73)	$\bar{3}m$	$3m$	$\bar{1}'$	$\bar{3}m$ χ=0	$3m$ $\begin{pmatrix} 0 & 0 & 0 & 0 & \chi_{15} & -\chi_{22} \\ -\chi_{22} & \chi_{22} & 0 & \chi_{15} & 0 & 0 \\ \chi_{31} & \chi_{31} & \chi_{33} & 0 & 0 & 0 \end{pmatrix}_4$	×
$\bar{3}'m'$ (20.4.74)	$\bar{3}m$	32	$\bar{1}'$	$\bar{3}m$ χ=0	32 $\begin{pmatrix} \chi_{11} & -\chi_{11} & 0 & \chi_{14} & 0 & 0 \\ 0 & 0 & 0 & 0 & -\chi_{14} & -\chi_{11} \\ 0 & 0 & 0 & 0 & 0 & 0 \end{pmatrix}_2$	×
$\bar{3}m'$ (20.5.75)	$\bar{3}m$	$\bar{3}$	$2'_{100}$	$\bar{3}m$ χ=0	$\bar{3}m$ χ=0	✓
$6'$ (21.3.78)	6	3	$2'$	6 $\begin{pmatrix} 0 & 0 & 0 & \chi_{14} & \chi_{15} & 0 \\ 0 & 0 & 0 & \chi_{15} & -\chi_{14} & 0 \\ \chi_{31} & \chi_{31} & \chi_{33} & 0 & 0 & 0 \end{pmatrix}_4$	$\bar{6}$ $\begin{pmatrix} \chi_{11} & -\chi_{11} & 0 & 0 & 0 & -\chi_{22} \\ -\chi_{22} & \chi_{22} & 0 & 0 & 0 & -\chi_{11} \\ 0 & 0 & 0 & 0 & 0 & 0 \end{pmatrix}_2$	×

Continued on next page

Suppl. Tab. V – continued from previous page

MPG M_0	**PG** G_0	S_0	R'	G_0 and $[\chi^{\text{even}}_{il}]_{3\times6}$	G_1 and $[\chi^{\text{odd}}_{il}]_{3\times6}$	**LMC**
$\bar{6}'$ (22.3.81)	$\bar{6}$	3	m'_{001}	$\bar{6}$ $\begin{pmatrix} \chi_{11} & -\chi_{11} & 0 & 0 & 0 & -\chi_{22} \\ -\chi_{22} & \chi_{22} & 0 & 0 & 0 & -\chi_{11} \\ 0 & 0 & 0 & 0 & 0 & 0 \end{pmatrix}_2$	6 $\begin{pmatrix} 0 & 0 & 0 & \chi_{14} & \chi_{15} & 0 \\ 0 & 0 & 0 & \chi_{15} & -\chi_{14} & 0 \\ \chi_{31} & \chi_{31} & \chi_{33} & 0 & 0 & 0 \end{pmatrix}_4$	×
$6'/m$ (23.3.84)	$6/m$	$\bar{6}$	$\bar{1}'$	$6/m$ $\chi{=}0$	$\bar{6}$ $\begin{pmatrix} \chi_{11} & -\chi_{11} & 0 & 0 & 0 & -\chi_{22} \\ -\chi_{22} & \chi_{22} & 0 & 0 & 0 & -\chi_{11} \\ 0 & 0 & 0 & 0 & 0 & 0 \end{pmatrix}_2$	×
$6/m'$ (23.4.85)	$6/m$	6	$\bar{1}'$	$6/m$ $\chi{=}0$	6 $\begin{pmatrix} 0 & 0 & 0 & \chi_{14} & \chi_{15} & 0 \\ 0 & 0 & 0 & \chi_{15} & -\chi_{14} & 0 \\ \chi_{31} & \chi_{31} & \chi_{33} & 0 & 0 & 0 \end{pmatrix}_4$	×
$6'/m'$ (23.5.86)	$6/m$	$\bar{3}$	m'_{001}	$6/m$ $\chi{=}0$	$6/m$ $\chi{=}0$	×
$6'22'$ (24.3.89)	622	32	$2'_{001}$	622 $\begin{pmatrix} 0 & 0 & 0 & \chi_{14} & 0 & 0 \\ 0 & 0 & 0 & 0 & -\chi_{14} & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 \end{pmatrix}_1$	$\bar{6}2m$ $\begin{pmatrix} \chi_{11} & -\chi_{11} & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & -\chi_{11} \\ 0 & 0 & 0 & 0 & 0 & 0 \end{pmatrix}_1$	×
$62'2'$ (24.4.90)	622	6	$2'_{100}$	622 $\begin{pmatrix} 0 & 0 & 0 & \chi_{14} & 0 & 0 \\ 0 & 0 & 0 & 0 & -\chi_{14} & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 \end{pmatrix}_1$	$6mm$ $\begin{pmatrix} 0 & 0 & 0 & 0 & \chi_{15} & 0 \\ 0 & 0 & 0 & \chi_{15} & 0 & 0 \\ \chi_{31} & \chi_{31} & \chi_{33} & 0 & 0 & 0 \end{pmatrix}_3$	✓
$6'mm'$ (25.3.93)	$6mm$	$3m$	$2'_{001}$	$6mm$ $\begin{pmatrix} 0 & 0 & 0 & 0 & \chi_{15} & 0 \\ 0 & 0 & 0 & \chi_{15} & 0 & 0 \\ \chi_{31} & \chi_{31} & \chi_{33} & 0 & 0 & 0 \end{pmatrix}_3$	$\bar{6}m2$ $\begin{pmatrix} 0 & 0 & 0 & 0 & 0 & -\chi_{22} \\ -\chi_{22} & \chi_{22} & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 \end{pmatrix}_1$	×
$6m'm'$ (25.4.94)	$6mm$	6	m'_{100}	$6mm$ $\begin{pmatrix} 0 & 0 & 0 & 0 & \chi_{15} & 0 \\ 0 & 0 & 0 & \chi_{15} & 0 & 0 \\ \chi_{31} & \chi_{31} & \chi_{33} & 0 & 0 & 0 \end{pmatrix}_3$	622 $\begin{pmatrix} 0 & 0 & 0 & \chi_{14} & 0 & 0 \\ 0 & 0 & 0 & 0 & -\chi_{14} & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 \end{pmatrix}_1$	✓
$\bar{6}'m'2$ (26.3.97)	$\bar{6}m2$	32	m'_{001}	$\bar{6}m2$ $\begin{pmatrix} 0 & 0 & 0 & 0 & 0 & -\chi_{22} \\ -\chi_{22} & \chi_{22} & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 \end{pmatrix}_1$	622 $\begin{pmatrix} 0 & 0 & 0 & \chi_{14} & 0 & 0 \\ 0 & 0 & 0 & 0 & -\chi_{14} & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 \end{pmatrix}_1$	×
$\bar{6}'m2'$ (26.4.98)	$\bar{6}m2$	$3m$	m'_{001}	$\bar{6}m2$ $\begin{pmatrix} 0 & 0 & 0 & 0 & 0 & -\chi_{22} \\ -\chi_{22} & \chi_{22} & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 \end{pmatrix}_1$	$6mm$ $\begin{pmatrix} 0 & 0 & 0 & 0 & \chi_{15} & 0 \\ 0 & 0 & 0 & \chi_{15} & 0 & 0 \\ \chi_{31} & \chi_{31} & \chi_{33} & 0 & 0 & 0 \end{pmatrix}_3$	×

Continued on next page

Suppl. Tab. V – continued from previous page

MPG M_0	**PG** G_0	S_0	R'	G_0 and $[\chi^{\text{even}}_{il}]_{3\times6}$	G_1 and $[\chi^{\text{odd}}_{il}]_{3\times6}$	**LMC**
$\bar{6}m'2'$ (26.5.99)	$\bar{6}m2$	$\bar{6}$	m'_{100}	$\bar{6}m2$ $\begin{pmatrix} 0 & 0 & 0 & 0 & 0 & -\chi_{22} \\ -\chi_{22} & \chi_{22} & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 \end{pmatrix}_1$	$\bar{6}2m$ $\begin{pmatrix} \chi_{11} & -\chi_{11} & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & -\chi_{11} \\ 0 & 0 & 0 & 0 & 0 & 0 \end{pmatrix}_1$	✓
$6/m'mm$ (27.3.102)	$6/mmm$	$6mm$	$\bar{1}'$	$6/mmm$ χ=0	$6mm$ $\begin{pmatrix} 0 & 0 & 0 & 0 & \chi_{15} & 0 \\ 0 & 0 & 0 & \chi_{15} & 0 & 0 \\ \chi_{31} & \chi_{31} & \chi_{33} & 0 & 0 & 0 \end{pmatrix}_3$	×
$6'/mmm'$ (27.4.103)	$6/mmm$	$\bar{6}m2$	$\bar{1}'$	$6/mmm$ χ=0	$\bar{6}m2$ $\begin{pmatrix} 0 & 0 & 0 & 0 & 0 & -\chi_{22} \\ -\chi_{22} & \chi_{22} & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 \end{pmatrix}_1$	×
$6'/m'mm'$ (27.5.104)	$6/mmm$	$\bar{3}m$	$6'_{001}$	$6/mmm$ χ=0	$6/mmm$ χ=0	×
$6/mm'm'$ (27.6.105)	$6/mmm$	$6/m$	$2'_{100}$	$6/mmm$ χ=0	$6/mmm$ χ=0	✓
$6/m'm'm'$ (27.7.106)	$6/mmm$	622	$\bar{1}'$	$6/mmm$ χ=0	622 $\begin{pmatrix} 0 & 0 & 0 & \chi_{14} & 0 & 0 \\ 0 & 0 & 0 & 0 & -\chi_{14} & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 \end{pmatrix}_1$	×
$m'\bar{3}'$ (29.3.111)	$m\bar{3}$	23	$\bar{1}'$	$m\bar{3}$ χ=0	23 $\begin{pmatrix} 0 & 0 & 0 & \chi_{14} & 0 & 0 \\ 0 & 0 & 0 & 0 & \chi_{14} & 0 \\ 0 & 0 & 0 & 0 & 0 & \chi_{14} \end{pmatrix}_1$	×
$4'32'$ (30.3.114)	432	23	$4'_{001}$	432 χ=0	$\bar{4}3m$ $\begin{pmatrix} 0 & 0 & 0 & \chi_{14} & 0 & 0 \\ 0 & 0 & 0 & 0 & \chi_{14} & 0 \\ 0 & 0 & 0 & 0 & 0 & \chi_{14} \end{pmatrix}_1$	×
$\bar{4}'3m'$ (31.3.117)	$\bar{4}3m$	23	$\bar{4}'_{001}$	$\bar{4}3m$ $\begin{pmatrix} 0 & 0 & 0 & \chi_{14} & 0 & 0 \\ 0 & 0 & 0 & 0 & \chi_{14} & 0 \\ 0 & 0 & 0 & 0 & 0 & \chi_{14} \end{pmatrix}_1$	432 χ=0	×
$m'\bar{3}'m$ (32.3.120)	$m\bar{3}m$	$\bar{4}3m$	$\bar{1}'$	$m\bar{3}m$ χ=0	$\bar{4}3m$ $\begin{pmatrix} 0 & 0 & 0 & \chi_{14} & 0 & 0 \\ 0 & 0 & 0 & 0 & \chi_{14} & 0 \\ 0 & 0 & 0 & 0 & 0 & \chi_{14} \end{pmatrix}_1$	×
$m\bar{3}m'$ (32.4.121)	$m\bar{3}m$	$m\bar{3}$	$4'_{100}$	$m\bar{3}m$ χ=0	$m\bar{3}m$ χ=0	×
$m'\bar{3}'m'$ (32.5.122)	$m\bar{3}m$	432	$\bar{1}'$	$m\bar{3}m$ χ=0	432 χ=0	×

Supplementary Note 4. SYMMETRY OF AXIAL TENSOR USING ISOMORPHIC GROUP METHOD

Suppl. Note 4.1. Symmetry analysis using isomorphic group method

The circular photogalvanic effect (CPGE) describes circular-polarization-light-induced photocurrent phenomenon, and it is a kind of optical rectification phenomenon. The CPGE coefficient β_{ij} is defined as:

$$\frac{\mathrm{d}j_i}{\mathrm{d}t} = \beta_{ij}(\omega)[\mathbf{E}(\omega) \times \mathbf{E}^*(\omega)]_j, \tag{S23}$$

where the subscript i is the direction of photocurrent, and the subscript j is the spread direction of circular-polarization light. Besides, Edelstein effect (inverse spin galvanic effect) α_{ij} describes a linear response of the magnetic polarization to a electric field:

$$M_i = \sum_j \alpha_{ij} E_j. \tag{S24}$$

The CPGE effect coefficient β_{ij} in Eq. (S23) and Edelstein effect susceptibility α_{ij} in Eq. (S24) are all 3×3 pseudo-tensors (axial tensor) which exist in systems without inversion symmetry. Because they obey similar symmetry constraint, we focus on the symmetry of CPGE β_{ij} in the following, and the results are also suitable to α_{ij}.

Similar to SHG susceptibilities, we can divide β_{ij} into even and odd parts

$$\beta_{ij}{=}\beta_{ij}^{\text{even}} + \beta_{ij}^{\text{odd}}. \tag{S25}$$

The unitary R and anti-unitary R' operations have the same restriction on tensor β^{even}:

$$R/R' : \beta^{\text{even}} = \det(R) R \beta^{\text{even}} R^{-1}, \tag{S26}$$

where $\det(R)$ is the determinant of operation R. The transformations of β^{odd} under the symmetry R and R' are

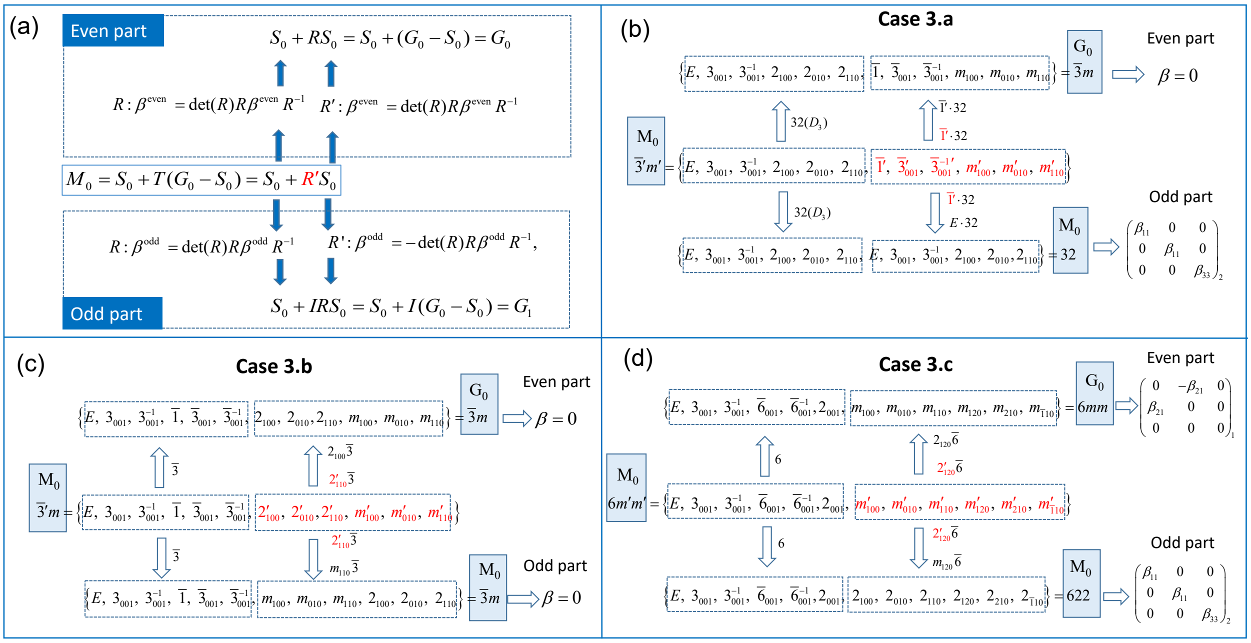
$$R/R' : \beta^{\text{odd}} = \pm \det(R) R \beta^{\text{odd}} R^{-1}, \tag{S27}$$

where the positive sign corresponds to the unitary operation R, while the minus sign corresponds to the anti-unitary operation R'.

Because $-1 = -(I_0)_{3\times 3}$ (I_0 is the identity matrix), i.e., -1 is identical to the matrix of inversion symmetry I, we can transform R' in Eq. (S27) as

$$\begin{aligned} R' : \beta^{\text{odd}} &= -\det(R) R \beta^{\text{odd}} R^{-1} \\ &= \det(-R)\,(-R)\,\beta^{\text{odd}}\left(-R^{-1}\right) \\ &= \det(IR)\,(IR)\,\beta^{\text{odd}}(IR)^{-1}, \end{aligned} \tag{S28}$$

i.e., anti-unitary operation R' is equivalent to an unitary operation IR for β^{odd}.



Supplementary Figure 2: Seeking the symmetry of axial tensor β in BW MPGs using the isomorphic group method. (a) Transformation of β_{ij}^{even} and β_{ij}^{odd} of BW MPG under unitary and anti-unitary operations, and corresponding isomorphic group. Examples for (b) BW MPG with PT symmetry, (c) BW MPG with P symmetry, (d) BW MPG without P nor PT symmetry.

Similar to the SHG tensors, we can study the symmetry of CPGE tensor β in every MPG using the isomorphic group method.

(1) For the original point group $M_0 = G_0$, there is no anti-unitary symmetry operation, and the β_{ij}^{even} and β_{ij}^{odd} have the same symmetry restriction.

(2) For the grey MPGs, $M_0 = G_0 + TG_0 = G_0 1'$ ($1'$: time-reversal symmetry), the combined restriction on R and R' leads to the vanish of β_{ij}^{odd}, and β_{ij}^{even} is restricted by G_0 equivalently.

(3) For the black-white groups $M_0 = G_0 + T(G_0 - S_0) = S_0 + R'S_0$, we can also divide them into three sub -cases:

(3.a) MPG M_0 has the PT symmetry. The β_{ij}^{even} vanishes, because $\bar{1}'$ (PT symmetry) acts as the inversion symmetry for β_{ij}^{even}. For the odd part, the symmetry constrain is equivalent to $G_1 = S_0 + (II)\, S_0 = S_0$, if $\bar{1}' \in R'S_0$.

(3.b) M_0 has the P symmetry. In this case, all of the even and odd CPGE tensors vanish due to existing inversion symmetry in M_0, and $G_1 = G_0$.

(3.c) M_0 has no P nor PT symmetry. In this case, both β_{ij}^{even} and β_{ij}^{odd} exist. Because the constraint of R' on the even part acts as an unitary operation R, the symmetry of β_{ij}^{even} under M_0 equals to isomorphism point group G_0. On the other hand, the constraint of β_{ij}^{odd} under M_0 is equivalent to point group $G_1 = S_0 + IRS_0$. Besides, $G_1 \neq G_0$ (because $\bar{1} \notin S_0$) and $G_1 \neq S_0$ (because $\bar{1}' \notin R'S_0$) in this case, i.e. G_0 and G_1 are the isomorphic relations.

See Figure 2 for the three specific examples of the above three subcases (3.a, 3.b, and 3.c). The axial tensors (CPGE tensors and Edelstein effect susceptibility tensor) in original and grey MPGs are summarized in Table VI, and the axial tensors of 58 BW MPGs are summarized in Table VII. The results are consistent with Refs. [9] and [7]; moreover, our method simplifies the tensor symmetries under magnetic point groups into nonmagnetic points groups efficiently and captures symmetry rules.

Suppl. Note 4.2. Axial tensor tables of original and grey MPGs

Suppl. Tab. VI: Axial tensors of original and grey magnetic point groups (MPGs) without inversion symmetry.

MPG M_0	**Axial tensor** $[\beta_{ij}]_{3\times3}$	**MPG** M_0	**Axial tensor** $[\beta_{ij}]_{3\times3}$
1 (1.1.1) $11'$ (1.2.2)	$\begin{pmatrix}\beta_{11}&\beta_{12}&\beta_{13}\\\beta_{21}&\beta_{22}&\beta_{23}\\\beta_{31}&\beta_{32}&\beta_{33}\end{pmatrix}_9$	3 (16.1.60) $31'$ (16.2.61)	$\begin{pmatrix}\beta_{11}&-\beta_{21}&0\\\beta_{21}&\beta_{11}&0\\0&0&\beta_{33}\end{pmatrix}_3$
2 (3.1.6) $21'$ (3.2.7)	$\begin{pmatrix}\beta_{11}&0&\beta_{13}\\0&\beta_{22}&0\\\beta_{31}&0&\beta_{33}\end{pmatrix}_5$	32 (18.1.65) $321'$ (18.2.66)	$\begin{pmatrix}\beta_{11}&0&0\\0&\beta_{11}&0\\0&0&\beta_{33}\end{pmatrix}_2$
m (4.1.9) $m1'$ (4.2.10)	$\begin{pmatrix}0&\beta_{12}&0\\\beta_{21}&0&\beta_{23}\\0&\beta_{32}&0\end{pmatrix}_4$	$3m$ (19.1.68) $3m1'$ (19.2.69)	$\begin{pmatrix}0&-\beta_{21}&0\\\beta_{21}&0&0\\0&0&0\end{pmatrix}_1$
222 (6.1.17) $2221'$ (6.2.18)	$\begin{pmatrix}\beta_{11}&0&0\\0&\beta_{22}&0\\0&0&\beta_{33}\end{pmatrix}_3$	6 (21.1.76) $61'$ (21.2.77)	$\begin{pmatrix}\beta_{11}&-\beta_{21}&0\\\beta_{21}&\beta_{11}&0\\0&0&\beta_{33}\end{pmatrix}_3$
$mm2$ (7.1.20) $mm21'$ (7.2.21)	$\begin{pmatrix}0&\beta_{12}&0\\\beta_{21}&0&0\\0&0&0\end{pmatrix}_2$	$\overline{6}$ (22.1.79) $\overline{6}1'$ (22.2.80)	β=0
4 (9.1.29) $41'$ (9.2.30)	$\begin{pmatrix}\beta_{11}&-\beta_{21}&0\\\beta_{21}&\beta_{11}&0\\0&0&\beta_{33}\end{pmatrix}_3$	622 (24.1.87) $6221'$ (24.2.88)	$\begin{pmatrix}\beta_{11}&0&0\\0&\beta_{11}&0\\0&0&\beta_{33}\end{pmatrix}_2$
$\overline{4}$ (10.1.32) $\overline{4}1'$ (10.2.33)	$\begin{pmatrix}\beta_{11}&\beta_{21}&0\\\beta_{21}&-\beta_{11}&0\\0&0&0\end{pmatrix}_2$	$6mm$ (25.1.91) $6mm1'$ (25.2.92)	$\begin{pmatrix}0&-\beta_{21}&0\\\beta_{21}&0&0\\0&0&0\end{pmatrix}_1$
422 (12.1.40) $4221'$ (12.2.41)	$\begin{pmatrix}\beta_{11}&0&0\\0&\beta_{11}&0\\0&0&\beta_{33}\end{pmatrix}_3$	$\overline{6}m2$ (26.1.95) $\overline{6}m21'$ (26.2.96)	β=0
$4mm$ (13.1.44) $4mm1'$ (13.2.45)	$\begin{pmatrix}0&-\beta_{21}&0\\\beta_{21}&0&0\\0&0&0\end{pmatrix}_1$	23 (28.1.107) $231'$ (28.2.108) 432 (30.1.112) $4321'$ (30.2.113)	$\begin{pmatrix}\beta_{11}&0&0\\0&\beta_{11}&0\\0&0&\beta_{11}\end{pmatrix}_1$
$\overline{4}2m$ (14.1.48) $\overline{4}2m1'$ (14.2.49)	$\begin{pmatrix}\beta_{11}&0&0\\0&-\beta_{11}&0\\0&0&0\end{pmatrix}_1$	$\overline{4}3m$ (31.1.115) $\overline{4}3m1'$ (31.2.116)	β=0

1. There is only the even part (β^{even}) for grey MPGs (the second one of each row, with $1'$), and the odd and even parts (β^{even}) and β^{odd}) have same symmetry in original MPGs (the first MPG of each row, without $1'$).
2. The subscript number of the tensor means the independent element number.
3. $[\beta_{ij}]_{3\times3}$ is zero for the original and grey groups not listed here because they have the inversion symmetry.

Suppl. Note 4.3. Axial tensor tables of all BW MPGs

Suppl. Tab. VII: Axial tensors of all BW MPGs. Note: (1) MPG $M_0 = S_0 + T(G_0 - S_0) = S_0 + R'S_0$, where G_0 is the isomorphism non-magnetic point group, and S_0 is the invariant subgroup of point group G_0 ($s = g/2$, s and g are the order of group S_0 and G_0 respectively). (2) The subscript number of each axial tensor means the independent element number.

MPG M_0	**Isomorphic PG** G_0	S_0	R'	G_0 and $[\beta_{ij}^{\text{even}}]_{3\times3}$	G_1 and $[\beta_{ij}^{\text{odd}}]_{3\times3}$
$\bar{1}'$ (2.3.5)	$\bar{1}$	1	$\bar{1}'$	$\bar{1}$ β=0	1 $\begin{pmatrix}\beta_{11} & \beta_{12} & \beta_{13}\\ \beta_{21} & \beta_{22} & \beta_{23}\\ \beta_{31} & \beta_{32} & \beta_{33}\end{pmatrix}_9$
$2'(2//y)$ (3.3.8)	2	1	$2'_{010}$	2 $\begin{pmatrix}\beta_{11} & 0 & \beta_{13}\\ 0 & \beta_{22} & 0\\ \beta_{31} & 0 & \beta_{33}\end{pmatrix}_5$	m $\begin{pmatrix}0 & \beta_{12} & 0\\ \beta_{21} & 0 & \beta_{23}\\ 0 & \beta_{32} & 0\end{pmatrix}_4$
$m'(m \perp y)$ (4.3.11)	$m(m\perp y)$	1	m'_{010}	m $\begin{pmatrix}0 & \beta_{12} & 0\\ \beta_{21} & 0 & \beta_{23}\\ 0 & \beta_{32} & 0\end{pmatrix}_4$	2 $\begin{pmatrix}\beta_{11} & 0 & \beta_{13}\\ 0 & \beta_{22} & 0\\ \beta_{31} & 0 & \beta_{33}\end{pmatrix}_5$
$2'/m(2//y)$ (5.3.14)	$2/m$	m	$\bar{1}'$	$2/m$ β=0	m $\begin{pmatrix}0 & \beta_{12} & 0\\ \beta_{21} & 0 & \beta_{23}\\ 0 & \beta_{32} & 0\end{pmatrix}_4$
$2/m'(2//y)$ (5.4.15)	$2/m$	2	$\bar{1}'$	$2/m$ β=0	2 $\begin{pmatrix}\beta_{11} & 0 & \beta_{13}\\ 0 & \beta_{22} & 0\\ \beta_{31} & 0 & \beta_{33}\end{pmatrix}_5$
$2'/m'(2//y)$ (5.5.16)	$2/m$	$\bar{1}$	$2'$	$2/m$ β=0	$2/m$ β=0
$2'2'2$ (6.3.19)	222	2 $(2//z)$	$2'_{100}$	222 $\begin{pmatrix}\beta_{11} & 0 & 0\\ 0 & \beta_{22} & 0\\ 0 & 0 & \beta_{33}\end{pmatrix}_3$	$mm2$ $\begin{pmatrix}0 & \beta_{12} & 0\\ \beta_{21} & 0 & 0\\ 0 & 0 & 0\end{pmatrix}_2$
$m'm2'(2//z)$ (7.3.22)	$mm2$	m $(m\perp y)$	$2'_{001}$	$mm2$ $\begin{pmatrix}0 & \beta_{12} & 0\\ \beta_{21} & 0 & 0\\ 0 & 0 & 0\end{pmatrix}_2$	$2mm$ $\begin{pmatrix}0 & 0 & 0\\ 0 & 0 & \beta_{32}\\ 0 & \beta_{23} & 0\end{pmatrix}_2$
$m'm'2$ (7.4.23)	$mm2$	2 $(2//z)$	m'_{100}	$mm2$ $\begin{pmatrix}0 & \beta_{12} & 0\\ \beta_{21} & 0 & 0\\ 0 & 0 & 0\end{pmatrix}_2$	222 $\begin{pmatrix}\beta_{11} & 0 & 0\\ 0 & \beta_{22} & 0\\ 0 & 0 & \beta_{33}\end{pmatrix}_3$

Continued on next page

Suppl. Tab. VII – continued from previous page

MPG M_0	**Isomorphic PG** G_0	S_0	R'	G_0 and $[\beta_{ij}^{\text{even}}]_{3\times3}$	G_1 and $[\beta_{ij}^{\text{odd}}]_{3\times3}$
mmm' (8.3.26)	mmm	$mm2$	$\bar{1}'$	mmm β=0	$mm2$ $\begin{pmatrix} 0 & \beta_{12} & 0 \\ \beta_{21} & 0 & 0 \\ 0 & 0 & 0 \end{pmatrix}_2$
$m'm'm$ (8.4.27)	mmm	$2/m(2//z)$	m'_{100}	mmm β=0	mmm β=0
$m'm'm'$ (8.5.28)	mmm	222	$\bar{1}'$	mmm β=0	222 $\begin{pmatrix} \beta_{11} & 0 & 0 \\ 0 & \beta_{22} & 0 \\ 0 & 0 & \beta_{33} \end{pmatrix}_3$
$4'$ (9.3.31)	4	2 $(2//z)$	$4'_{001}$	4 $\begin{pmatrix} \beta_{11} & -\beta_{21} & 0 \\ \beta_{21} & \beta_{11} & 0 \\ 0 & 0 & \beta_{33} \end{pmatrix}_3$	$\bar{4}$ $\begin{pmatrix} \beta_{11} & \beta_{21} & 0 \\ \beta_{21} & -\beta_{11} & 0 \\ 0 & 0 & 0 \end{pmatrix}_2$
$\bar{4}'$ (10.3.34)	$\bar{4}$	2 $(2//z)$	$\bar{4}'_{001}$	$\bar{4}$ $\begin{pmatrix} \beta_{11} & \beta_{21} & 0 \\ \beta_{21} & -\beta_{11} & 0 \\ 0 & 0 & 0 \end{pmatrix}_2$	4 $\begin{pmatrix} \beta_{11} & -\beta_{21} & 0 \\ \beta_{21} & \beta_{11} & 0 \\ 0 & 0 & \beta_{33} \end{pmatrix}_3$
$4'/m$ (11.3.37)	$4/m$	$2/m$	$4'_{001}$	$4/m$ β=0	$4/m$ β=0
$4/m'$ (11.4.38)	$4/m$	4	$\bar{1}'$	$4/m$ β=0	4 $\begin{pmatrix} \beta_{11} & -\beta_{21} & 0 \\ \beta_{21} & \beta_{11} & 0 \\ 0 & 0 & \beta_{33} \end{pmatrix}_3$
$4'/m'$ (11.5.39)	$4/m$	$\bar{4}$	$\bar{1}'$	$4/m$ β=0	$\bar{4}$ $\begin{pmatrix} \beta_{11} & \beta_{21} & 0 \\ \beta_{21} & -\beta_{11} & 0 \\ 0 & 0 & 0 \end{pmatrix}_2$
$4'22'$ (12.3.42)	422	222	$4'_{001}$	422 $\begin{pmatrix} \beta_{11} & 0 & 0 \\ 0 & \beta_{11} & 0 \\ 0 & 0 & \beta_{33} \end{pmatrix}_3$	$\bar{4}2m$ $\begin{pmatrix} \beta_{11} & 0 & 0 \\ 0 & -\beta_{11} & 0 \\ 0 & 0 & 0 \end{pmatrix}_1$
$42'2'$ (12.4.43)	422	4	$2'_{100}$	422 $\begin{pmatrix} \beta_{11} & 0 & 0 \\ 0 & \beta_{11} & 0 \\ 0 & 0 & \beta_{33} \end{pmatrix}_3$	$4mm$ $\begin{pmatrix} 0 & -\beta_{21} & 0 \\ \beta_{21} & 0 & 0 \\ 0 & 0 & 0 \end{pmatrix}_1$
$4'm'm$ (13.3.46)	$4mm$	$2mm$	$4'_{001}$	$4mm$ $\begin{pmatrix} 0 & -\beta_{21} & 0 \\ \beta_{21} & 0 & 0 \\ 0 & 0 & 0 \end{pmatrix}_1$	$\bar{4}2m$ $\begin{pmatrix} \beta_{11} & 0 & 0 \\ 0 & -\beta_{11} & 0 \\ 0 & 0 & 0 \end{pmatrix}_1$

Continued on next page

Suppl. Tab. VII – continued from previous page

MPG M_0	Isomorphic PG G_0	S_0	R'	G_0 and $[\beta_{ij}^{\text{even}}]_{3\times3}$	G_1 and $[\beta_{ij}^{\text{odd}}]_{3\times3}$
$4m'm'$ (13.4.47)	$4mm$	4	m'_{100}	$4mm$ $\begin{pmatrix} 0 & -\beta_{21} & 0 \\ \beta_{21} & 0 & 0 \\ 0 & 0 & 0 \end{pmatrix}_1$	422 $\begin{pmatrix} \beta_{11} & 0 & 0 \\ 0 & \beta_{11} & 0 \\ 0 & 0 & \beta_{33} \end{pmatrix}_3$
$\bar{4}'2'm$ (14.3.50)	$\bar{4}2m$	$2mm$	$\bar{4}'$	$\bar{4}2m$ $\begin{pmatrix} \beta_{11} & 0 & 0 \\ 0 & -\beta_{11} & 0 \\ 0 & 0 & 0 \end{pmatrix}_1$	$4mm$ $\begin{pmatrix} 0 & -\beta_{21} & 0 \\ \beta_{21} & 0 & 0 \\ 0 & 0 & 0 \end{pmatrix}_1$
$\bar{4}'2m'$ (14.4.51)	$\bar{4}2m$	222	$\bar{4}'$	$\bar{4}2m$ $\begin{pmatrix} \beta_{11} & 0 & 0 \\ 0 & -\beta_{11} & 0 \\ 0 & 0 & 0 \end{pmatrix}_1$	422 $\begin{pmatrix} \beta_{11} & 0 & 0 \\ 0 & \beta_{11} & 0 \\ 0 & 0 & \beta_{33} \end{pmatrix}_3$
$\bar{4}2'm'$ (14.5.52)	$\bar{4}2m$	$\bar{4}$	$2'_{100}$	$\bar{4}2m$ $\begin{pmatrix} \beta_{11} & 0 & 0 \\ 0 & -\beta_{11} & 0 \\ 0 & 0 & 0 \end{pmatrix}_1$	$\bar{4}m2$ $\begin{pmatrix} 0 & \beta_{12} & 0 \\ \beta_{12} & 0 & 0 \\ 0 & 0 & 0 \end{pmatrix}_1$
$4/m'mm$ (15.3.55)	$4/mmm$	$4mm$	$\bar{1}'$	$4/mmm$ β=0	$4mm$ $\begin{pmatrix} 0 & -\beta_{21} & 0 \\ \beta_{21} & 0 & 0 \\ 0 & 0 & 0 \end{pmatrix}_1$
$4'/mm'm$ (15.4.56)	$4/mmm$	mmm	$\bar{4}'$	$4/mmm$ β=0	$4/mmm$ β=0
$4'/m'm'm$ (15.5.57)	$4/mmm$	$\bar{4}2m$	$\bar{1}'$	$4/mmm$ β=0	$\bar{4}2m$ $\begin{pmatrix} \beta_{11} & 0 & 0 \\ 0 & -\beta_{11} & 0 \\ 0 & 0 & 0 \end{pmatrix}_1$
$4/mm'm'$ (15.6.58)	$4/mmm$	$4/m$	$2'_{100}$	$4/mmm$ β=0	$4/mmm$ β=0
$4/m'm'm'$ (15.7.59)	$4/mmm$	422	$\bar{1}'$	$4/mmm$ β=0	422 $\begin{pmatrix} \beta_{11} & 0 & 0 \\ 0 & \beta_{11} & 0 \\ 0 & 0 & \beta_{33} \end{pmatrix}_3$
$\bar{3}'$ (17.3.64)	$\bar{3}$	3	$\bar{1}'$	$\bar{3}$ β=0	3 $\begin{pmatrix} \beta_{11} & -\beta_{21} & 0 \\ \beta_{21} & \beta_{11} & 0 \\ 0 & 0 & \beta_{33} \end{pmatrix}_3$
$32'$ (18.3.67)	32	3	$2'_{100}$	32 $\begin{pmatrix} \beta_{11} & 0 & 0 \\ 0 & \beta_{11} & 0 \\ 0 & 0 & \beta_{33} \end{pmatrix}_2$	$3m$ $\begin{pmatrix} 0 & -\beta_{21} & 0 \\ \beta_{21} & 0 & 0 \\ 0 & 0 & 0 \end{pmatrix}_1$

Continued on next page

Suppl. Tab. VII – continued from previous page

MPG M_0	Isomorphic PG G_0	S_0	R'	G_0 and $[\beta_{ij}^{\text{even}}]_{3\times 3}$	G_1 and $[\beta_{ij}^{\text{odd}}]_{3\times 3}$
$3m'$ (19.3.70)	$3m$	3	m'_{100}	$3m$ $\begin{pmatrix} 0 & -\beta_{21} & 0 \\ \beta_{21} & 0 & 0 \\ 0 & 0 & 0 \end{pmatrix}_1$	32 $\begin{pmatrix} \beta_{11} & 0 & 0 \\ 0 & \beta_{11} & 0 \\ 0 & 0 & \beta_{33} \end{pmatrix}_2$
$\overline{3}'m$ (20.3.73)	$\overline{3}m$	$3m$	$\overline{1}'$	$\overline{3}m$ $\beta{=}0$	$3m$ $\begin{pmatrix} 0 & -\beta_{21} & 0 \\ \beta_{21} & 0 & 0 \\ 0 & 0 & 0 \end{pmatrix}_1$
$\overline{3}'m'$ (20.4.74)	$\overline{3}m$	32	$\overline{1}'$	$\overline{3}m$ $\beta{=}0$	32 $\begin{pmatrix} \beta_{11} & 0 & 0 \\ 0 & \beta_{11} & 0 \\ 0 & 0 & \beta_{33} \end{pmatrix}_2$
$\overline{3}m'$ (20.5.75)	$\overline{3}m$	$\overline{3}$	$2'_{100}$	$\overline{3}m$ $\beta{=}0$	$\overline{3}m$ $\beta{=}0$
$6'$ (21.3.78)	6	3	$2'$	6 $\begin{pmatrix} \beta_{11} & -\beta_{21} & 0 \\ \beta_{21} & \beta_{11} & 0 \\ 0 & 0 & \beta_{33} \end{pmatrix}_3$	$\overline{6}$ $\beta{=}0$
$\overline{6}'$ (22.3.81)	$\overline{6}$	3	m'_{001}	$\overline{6}$ $\beta{=}0$	6 $\begin{pmatrix} \beta_{11} & -\beta_{21} & 0 \\ \beta_{21} & \beta_{11} & 0 \\ 0 & 0 & \beta_{33} \end{pmatrix}_3$
$6'/m$ (23.3.84)	$6/m$	$\overline{6}$	$\overline{1}'$	$6/m$ $\beta{=}0$	$\overline{6}$ $\beta{=}0$
$6/m'$ (23.4.85)	$6/m$	6	$\overline{1}'$	$6/m$ $\beta{=}0$	6 $\begin{pmatrix} \beta_{11} & -\beta_{21} & 0 \\ \beta_{21} & \beta_{11} & 0 \\ 0 & 0 & \beta_{33} \end{pmatrix}_3$
$6'/m'$ (23.5.86)	$6/m$	$\overline{3}$	m'_{001}	$6/m$ $\beta{=}0$	$6/m$ $\beta{=}0$
$6'22'$ (24.3.89)	622	32	$2'_{001}$	622 $\begin{pmatrix} \beta_{11} & 0 & 0 \\ 0 & \beta_{11} & 0 \\ 0 & 0 & \beta_{33} \end{pmatrix}_2$	$\overline{6}2m$ $\beta{=}0$
$62'2'$ (24.4.90)	622	6	$2'_{100}$	622 $\begin{pmatrix} \beta_{11} & 0 & 0 \\ 0 & \beta_{11} & 0 \\ 0 & 0 & \beta_{33} \end{pmatrix}_2$	$6mm$ $\begin{pmatrix} 0 & -\beta_{21} & 0 \\ \beta_{21} & 0 & 0 \\ 0 & 0 & 0 \end{pmatrix}_1$

Continued on next page

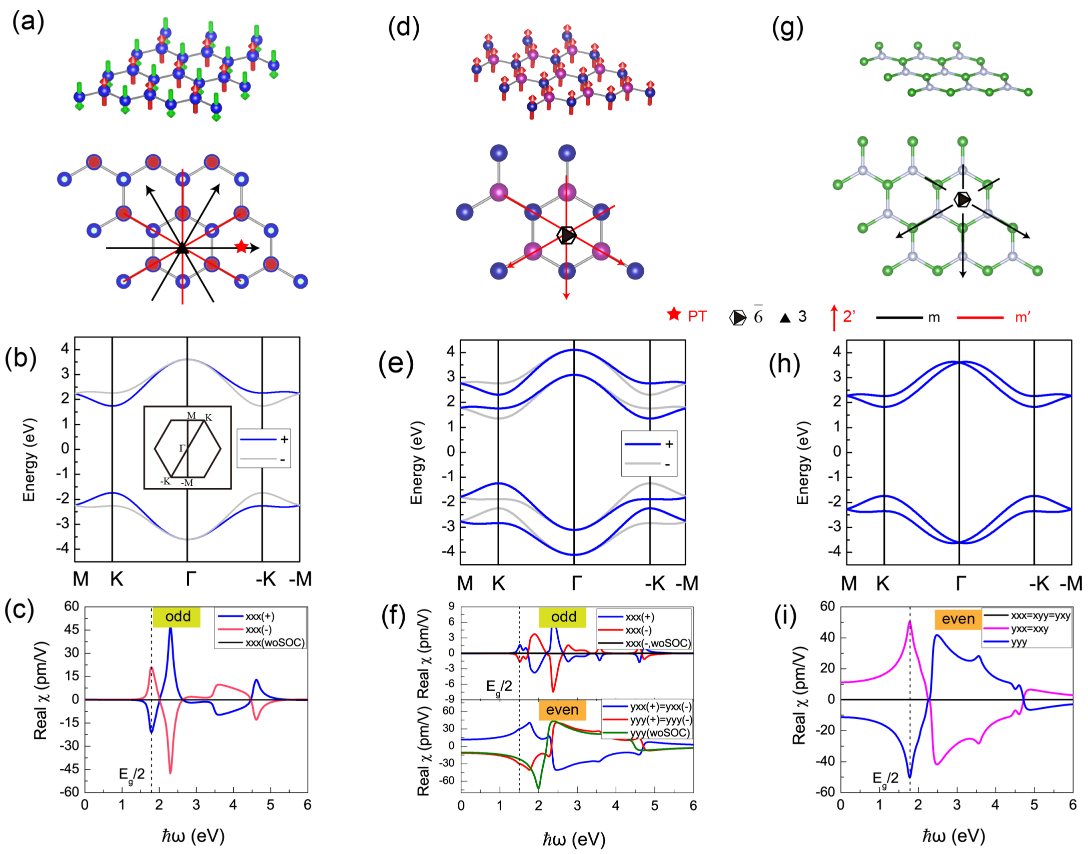
Suppl. Tab. VII – continued from previous page

MPG M_0	Isomorphic PG G_0	S_0	R'	G_0 and $[\beta_{ij}^{\text{even}}]_{3\times3}$	G_1 and $[\beta_{ij}^{\text{odd}}]_{3\times3}$
$6'mm'$ (25.3.93)	$6mm$	$3m$	$2'_{001}$	$6mm$ $\begin{pmatrix} 0 & -\beta_{21} & 0 \\ \beta_{21} & 0 & 0 \\ 0 & 0 & 0 \end{pmatrix}_1$	$\bar{6}m2$ $\beta{=}0$
$6m'm'$ (25.4.94)	$6mm$	6	m'_{100}	$6mm$ $\begin{pmatrix} 0 & -\beta_{21} & 0 \\ \beta_{21} & 0 & 0 \\ 0 & 0 & 0 \end{pmatrix}_1$	622 $\begin{pmatrix} \beta_{11} & 0 & 0 \\ 0 & \beta_{11} & 0 \\ 0 & 0 & \beta_{33} \end{pmatrix}_2$
$\bar{6}'m'2$ (26.3.97)	$\bar{6}m2$	32	m'_{001}	$\bar{6}m2$ $\beta{=}0$	622 $\begin{pmatrix} \beta_{11} & 0 & 0 \\ 0 & \beta_{11} & 0 \\ 0 & 0 & \beta_{33} \end{pmatrix}_2$
$\bar{6}'m2'$ (26.4.98)	$\bar{6}m2$	$3m$	m'_{001}	$\bar{6}m2$ $\beta{=}0$	$6mm$ $\begin{pmatrix} 0 & -\beta_{21} & 0 \\ \beta_{21} & 0 & 0 \\ 0 & 0 & 0 \end{pmatrix}_1$
$\bar{6}m'2'$ (26.5.99)	$\bar{6}m2$	$\bar{6}$	m'_{100}	$\bar{6}m2$ $\beta{=}0$	$\bar{6}2m$ $\beta{=}0$
$6/m'mm$ (27.3.102)	$6/mmm$	$6mm$	$\bar{1}'$	$6/mmm$ $\beta{=}0$	$6mm$ $\begin{pmatrix} 0 & -\beta_{21} & 0 \\ \beta_{21} & 0 & 0 \\ 0 & 0 & 0 \end{pmatrix}_1$
$6'/mmm'$ (27.4.103)	$6/mmm$	$\bar{6}m2$	$\bar{1}'$	$6/mmm$ $\beta{=}0$	$\bar{6}m2$ $\beta{=}0$
$6'/m'mm'$ (27.5.104)	$6/mmm$	$\bar{3}m$	$6'_{001}$	$6/mmm$ $\beta{=}0$	$6/mmm$ $\beta{=}0$
$6/mm'm'$ (27.6.105)	$6/mmm$	$6/m$	$2'_{100}$	$6/mmm$ $\beta{=}0$	$6/mmm$ $\beta{=}0$
$6/m'm'm'$ (27.7.106)	$6/mmm$	622	$\bar{1}'$	$6/mmm$ $\beta{=}0$	622 $\begin{pmatrix} \beta_{11} & 0 & 0 \\ 0 & \beta_{11} & 0 \\ 0 & 0 & \beta_{33} \end{pmatrix}_2$
$m'\bar{3}'$ (29.3.111)	$m\bar{3}$	23	$\bar{1}'$	$m\bar{3}$ $\beta{=}0$	23 $\begin{pmatrix} \beta_{11} & 0 & 0 \\ 0 & \beta_{11} & 0 \\ 0 & 0 & \beta_{11} \end{pmatrix}_1$
$4'32'$ (30.3.114)	432	23	$4'_{001}$	432 $\begin{pmatrix} \beta_{11} & 0 & 0 \\ 0 & \beta_{11} & 0 \\ 0 & 0 & \beta_{11} \end{pmatrix}_1$	$\bar{4}3m$ $\beta{=}0$

Continued on next page

Suppl. Tab. VII – continued from previous page

MPG M_0	Isomorphic PG G_0	S_0	R'	G_0 and $[\beta_{ij}^{\mathrm{even}}]_{3\times3}$	G_1 and $[\beta_{ij}^{\mathrm{odd}}]_{3\times3}$
$\bar{4}'3m'$ (31.3.117)	$\bar{4}3m$	23	$\bar{4}'_{001}$	$\bar{4}3m$ β=0	432 $\begin{pmatrix}\beta_{11} & 0 & 0\\ 0 & \beta_{11} & 0\\ 0 & 0 & \beta_{11}\end{pmatrix}_1$
$m'\bar{3}'m$ (32.3.120)	$m\bar{3}m$	$\bar{4}3m$	$\bar{1}'$	$m\bar{3}m$ β=0	$\bar{4}3m$ β=0
$m\bar{3}m'$ (32.4.121)	$m\bar{3}m$	$m\bar{3}$	$4'_{100}$	$m\bar{3}m$ β=0	$m\bar{3}m$ β=0
$m'\bar{3}'m'$ (32.5.122)	$m\bar{3}m$	432	$\bar{1}'$	$m\bar{3}m$ β=0	432 $\begin{pmatrix}\beta_{11} & 0 & 0\\ 0 & \beta_{11} & 0\\ 0 & 0 & \beta_{11}\end{pmatrix}_1$



Supplementary Figure 3: SHG results of the effective model with 2D honeycomb lattice. (a) Crystal structure, (b) band structures, and (c) SHG (with PT-wP type) susceptibilities of Néel AFM with PT symmetry. (d) Crystal structure, (e) band structures, and (f) SHG (with BW-woP type) susceptibilities of FM without sub-lattice symmetry ($\lambda_V = 2$ eV here). (d) Crystal structure, (e) band structures, and (f) SHG susceptibilities of nonmagnetic lattice ($\lambda_M = 0$) without sub-lattice symmetry. The real and imaginary parts of SHG share the same symmetry, and the imaginary parts are not shown. The "+" and "−" signs in (c) and (f) represent the positive and negative magnetic structures.

Supplementary Note 5. SUPPLEMENTARY CALCULATIONS AND DISSCUSSION

Suppl. Note 5.1. SHG of effect models with a honeycomb lattice

Here, we consider effect models with honeycomb lattice to explore the SHG types under magnetic groups, and the effect of magnetic moment and spin-orbit coupling (SOC) effect on SHG. To describe a Néel AFM magnetic structure with PT symmetry, as shown in Figure 3(a) (with MSG of $P6'/mm'm$). We use the following 4-bands Kane-Mele model [17] to describe it.

$$H = t\sum_{\langle ij\rangle\alpha} c_{i\alpha}^{\dagger} c_{j\alpha} + \lambda_M \sum_{i} (-1)^i c_i^{\dagger} s^z c_i + i\lambda_{\text{SO}} \sum_{\langle\langle ij\rangle\rangle} \nu_{ij} c_i^{\dagger} s^z c_j. \tag{S29}$$

The first term in Eq. (S29) is the nearest neighbor hopping, the second is the exchange Zeeman field, mimicking the Néel order with an out-of-plane easy axis, and the third term is the intrinsic SOC effect. Here, $v_{ij} = \left(2/\sqrt{3}\,\right)(\mathbf{d}_1 \times \mathbf{d}_1) = \pm 1$, where $\mathbf{d}_1$ and $\mathbf{d}_2$ are the unit vectors of the two bonds connecting site i to j, and s^z is the spin Pauli matrix. $t = 1$ eV, $\lambda_M = 2$ eV, and $\lambda_{\text{SO}} = 0.05$ eV, here. Due to the PT symmetry, the band structures are double degenerate as shown in Figure 3(b). Besides, the time-reversal symmetry is broken as a result of the coupling of SOC effect and magnetism, and +K and -K valleys are nonequivalent [18, 19].

The SHG type of this Néel AFM belongs to the PT-wP according to our classification, where only the odd

SHG parts exist. Its tensor is constrained by point group $\bar{6}2m$ (D_{3h}) according to the above symmetry analysis. The calculated nonzero SHG tensor elements are $\chi^{\text{odd}}_{xxx} = -\chi^{\text{odd}}_{xyy} = -\chi^{\text{odd}}_{yxy} = -\chi^{\text{odd}}_{yyx}$, as shown in Figure 3(b). By switching the sign of λ_M in Eq. (S29) to reverse the magnetic moments, and we find all the nonzero SHG tensor elements reverse accordingly, which is consistent with our symmetry analysis. The recently studied CrI_3 [20–22], $MnPS_3$ [23], $MnPSe_3$ [24], $MnBi_2Te_4$ [25], and CrSBr [26] also have the similar SHG character of the model in Eq. (S29), because they belong to the same SHG types (PT-wP). The SHG responses in PT-wP are non-reciprocal, and are reversible by rotating magnetization direction. Besides, without the SOC effect [in Eq. (S29)], the odd parts SHG vanish. This indicates that the SOC effect plays an important role in the SHG of magnetic materials. The stronger SOC makes the SHG contribute by magnetism more significant, such as CrI_3 [21, 22] and $MnBi_2Te_4$ [25].

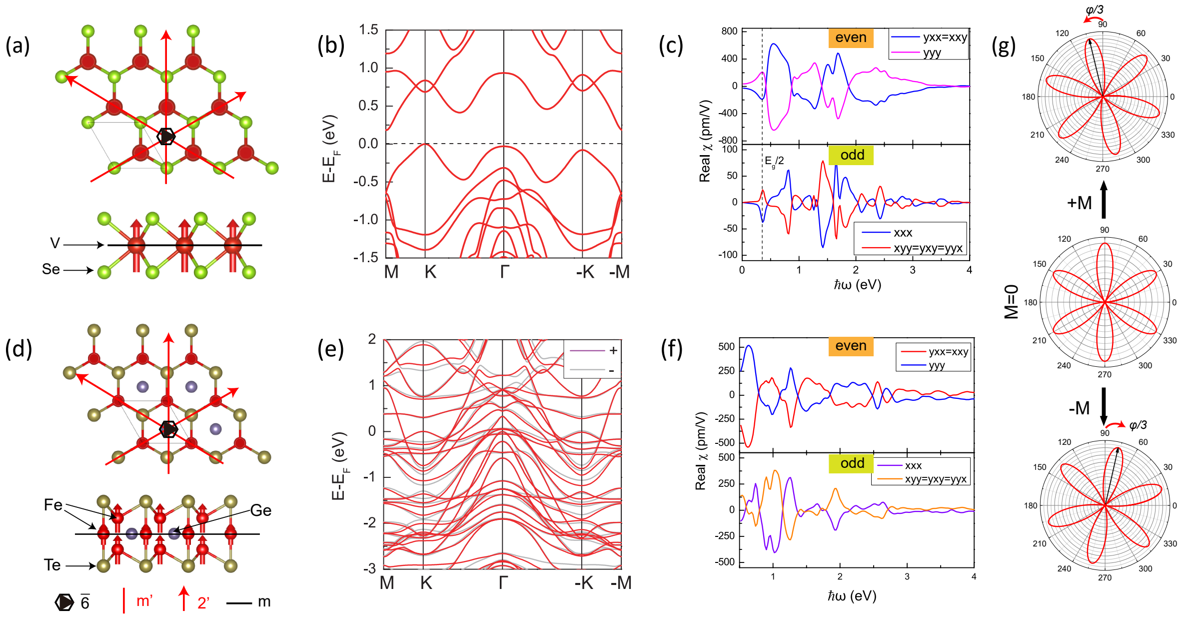
The 2D ferromagnetic honeycomb model without sub-lattice inversion symmetry (with $P\bar{6}m'2'$ symmetry, as shown in Figure 3(d)) can be written as [27]

$$\begin{aligned} H &= t \sum_{\langle ij\rangle\alpha} c^\dagger_{i\alpha} c_{j\alpha} + \lambda_M \sum_i (-1)^i c^\dagger_i s^0 c_i + \lambda_V \sum_i (-1)^i c^\dagger_i s^0 c_i \\ &+ i\lambda_{\text{SO}} \sum\nolimits_{\langle\langle ij\rangle\rangle} \nu_{ij} c^\dagger_i s^z c_j + i\lambda_R \sum_{\langle ij\rangle} c^\dagger_i \left(\mathbf{s} \times \hat{\mathbf{d}}_{ij}\right)_z c_j. \end{aligned} \tag{S30}$$

The second term is the exchange Zeeman field which is different from Eq. (S29), because it describes an FM exchange field. The third term breaks the sub-lattice inversion symmetry. The terms in the second line describe the SOC effect, and the first one is also presented in Eq. (S29), and the second one describes the Rashba SOC effect, which is essential to get the nonzero SHG for 4-band model [28]. t=1.0 eV, $\lambda_V = 1.0$ eV, $\lambda_M = 0.5$ eV, $\lambda_R = 0.2$ eV, and $\lambda_{\text{SO}} = 0.05$ eV, here. Due to the lacking of inversion symmetry and ferromagnetism, the bands split, as shown in Figure 3(e). According to its symmetry, we can judge its SHG type belongs to BW-woP, where the even and odd SHG coexist. The even parts SHG are constrained by the $G_0 = \bar{6}m2$ symmetry, leading to $\chi^{\text{even}}_{yyy} = -\chi^{\text{even}}_{yxx} = -\chi^{\text{even}}_{xyx} = -\chi^{\text{even}}_{xxy}$. While the odd parts are constrained by the $G_1 = \bar{6}2m$ point group, and $\chi^{\text{odd}}_{xxx} = -\chi^{\text{odd}}_{xyy} = -\chi^{\text{odd}}_{yxy} = -\chi^{\text{odd}}_{yyx}$ (the others are all zeros). The odd and even parts of tensor elements mutually repulse each other, because they are constrained by different symmetries. The calculated SHG results are shown in Figure 3(f), which are consistent with our symmetry analysis. At the zero frequency limits, the even parts of SHG are nonzero, while the odd parts are zero, as shown in Figure 3(f). Besides, the even SHG susceptibilities are invariant when the magnetism switches ($\lambda_M \to -\lambda_M$), while the odd parts reverse. Without the SOC effect [the fourth and fifth terms of Eq. (S30) are zeros], the odd parts of SHG become zeros, while the even parts of SHG survive.

The SG of the parent phase has no inversion symmetry, so the structure asymmetry contributes to the even parts of SHG, and can survive without magnetism. If $\lambda_M = 0$ in Eq. (S30), and it becomes a nonmagnetic 2D model without inversion symmetry, as shown in Figure 3(g). Its band structures are shown in Figure 3(h), where the band splits originate from the SOC effect and symmetry breaking of crystal structure. The band energies of $+\mathbf{k}$ and $-\mathbf{k}$ points are equivalent because the time-reversal symmetry links these two $\mathbf{k}$ points. Only the even parts of the SHG survive, as shown in Figure 3(i). Comparing Figure 3(f) with Figure 3(i), we find the magnitude of even parts SHG also are varied when λ_M is changed from nonzero to zero, therefore the magnetism contributes not only the odd parts of SHG but also the even parts.

Suppl. Note 5.2. Monolayer VSe_2 and Fe_3GeTe_2 with BW-woP SHG



Supplementary Figure 4: Calculation results of monolayer VSe_2 and Fe_3GeTe_2. (a) Crystal structure and (b) band structure of VSe_2, and corresponding (c) even and odd of SHG (with BW-woP type) tensor. (d) Crystal structure and (e) band structure of Fe_3GeTe_2, and corresponding (f) even and odd of SHG (with BW-woP type) tensor. (g) Polarization-resolved SHG signal $I_{//}$ (SHG signal is parallel with incident polarized light) with magnetism order. $\chi^{\text{even}}(\pm\mathbf{M})$: $\chi^{\text{odd}}(\pm\mathbf{M}) = 1 : \pm 0.8$, here.

As shown in Figure 4(a), monolayer $1H$-VSe_2 [19] has MSG of $P\bar{6}m'2'$ without inversion symmetry. Besides, its parent phase also has no inversion symmetry (with SG of $P\bar{6}m2$), leading to the BW-woP type of SHG. Due to the spin-orbit coupling (SOC) effect and magnetism, valence-band maximums (VBMs) at +K and -K are nonequivalent as shown in 4(b), resulting in valley polarization [19]. The even parts SHG are constrained by G_0=$\bar{6}m2$, hence $\chi^{\text{even}}_{yyy} = -\chi^{\text{even}}_{yxx} = -\chi^{\text{even}}_{xyx} = -\chi^{\text{even}}_{xxy} = \chi^{\text{even}}_{22}$. Besides, the odd part is restricted by G_1=$\bar{6}2m$, resulting in $\chi^{\text{odd}}_{xxx} = -\chi^{\text{odd}}_{xyy} = -\chi^{\text{odd}}_{yxy} = -\chi^{\text{odd}}_{yyx} = \chi^{\text{odd}}_{11}$. The calculated SHG susceptibilities are consistent with the above symmetry, as shown in Figure 4(c). The classification also indicates that the even SHG tensor elements are invariant when the magnetism is switched, while the odd parts reverse, consisting with our calculation results.

Monolayer Fe_3GeTe_2 is a 2D ferromagnetic metal, which was successfully synthesized in experiment [29]. As shown in Figure 4(d), its MSG is $P\bar{6}m'2'$ and its parent phase also has no inversion symmetry, which shares the same SHG type with monolayer VSe_2 (BW-woP type of SHG). The band structures are shown in Figure 4(e). The calculated SHG symmetries are consistent with that of monolayer VSe_2, as shown in Figure 4(f). We find the odd parts of SHG are in the same order as the even parts, due to the stronger SOC effect in monolayer Fe_3GeTe_2 than that of monolayer VSe_2. Bulk VSe_2 and bulk Fe_3GeTe_2 have no SHG effect due to the existence of inversion symmetry via interlayer stacking [30].

The studies of symmetries and origins help to characterize the magnetism and magnetic domains of these 2D materials with SHG. Parts of SHG tensor elements reversing with magnetic order are one of the features of the BW-woP type SHG, which will lead to unique SHG phenomena in experiments. The angle-dependent SHG patterns are simulated, and the polarization-resolved SHG signal $I_{//}$ is shown in Figure 4(g). Combining the even and odd parts, the total SHG tensors of monolayer VSe_2 and Fe_3GeTe_2 show $\bar{6}$ symmetry, according to symmetry analysis, leading to the misalignment of $I_{//}$ with x or y axis for +M and −M states. For ±M states, $I_{//}(\pm M) = \left(\chi_{11}^{\text{odd}}\cos 3\theta \mp \chi_{22}^{\text{even}}\sin 3\theta\right)^2 = \left[\left(\chi_{11}^{\text{odd}}\right)^2 + \left(\chi_{22}^{\text{even}}\right)^2\right][\sin(3\theta \mp \varphi)]^2$, where $\varphi = \arctan\left(\frac{\chi_{11}^{\text{odd}}}{\chi_{22}^{\text{even}}}\right)$. The odd SHG parts vanish when the magnetism disappears (M=0), and $I_{//} = (\chi_{22}^{\text{even}}\sin 3\theta)^2$. When the magnetic structure switches from +M to -M, the even SHG tensor elements keep invariant, while the odd parts reverse, leading to the SHG patterns rotates as shown in Figure 4(g). We can use the rotation angle $\varphi/3$ to speculate the relative magnitude of $\frac{\chi_{11}^{\text{odd}}}{\chi_{22}^{\text{even}}}$. The feature of the BW-woP type SHG is quite different from that of PT-wP type SHG, in which SHG patterns of two opposite magnetic orders are identical.

Suppl. Note 5.3. Magnetic and band structures, SHG and LMO characters of $YMnO_3$

The crystal structure of $RMnO_3$ (R = Y, Sc, In, Ho, Er, Tm, Lu, Yb) is shown in Table VIII, R atoms occupy $2a$ and $4b$ positions, Mn atoms occupy the $6c$ positions, and O atoms are at $6c$ positions. The magnetic structures of different magnetic phases are summarized in Table IX. The crystal structure of $YMnO_3$ refers to Ref. [31]. The band structures of $YMnO_3$ with different phases are shown in Figure 5, where there are little differences among them, except for the degenerate and non-degenerate bands.

Suppl. Tab. VIII: Wyckoff Positions of space group $P6_3cm$ (No. 185)

Multiplicity	Wyckoff letter	Site Symmetry	Position
6	c	$.m.$	(x,0,z) (0,x,z) (-x,-x,z) (-x,0,z+1/2) (0,-x,z+1/2) (x,x,z+1/2)
4	b	3..	(1/3,2/3,z) (2/3,1/3,z+1/2) (1/3,2/3,z+1/2) (2/3,1/3,z)
2	a	$3m$	(0,0,z) (0,0,z+1/2)

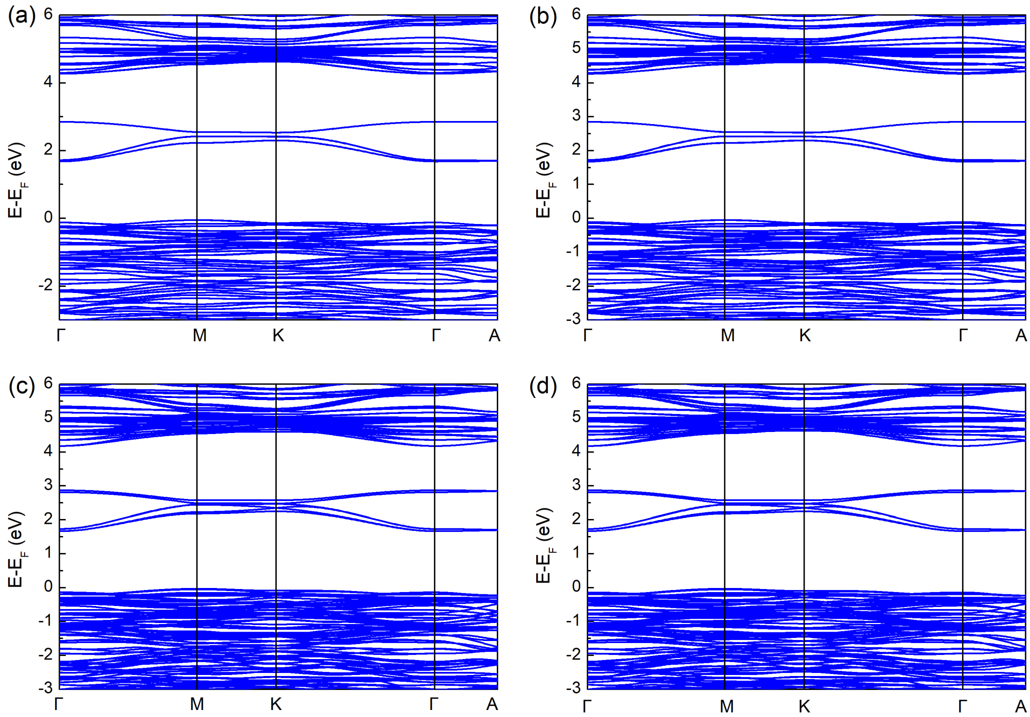
Suppl. Tab. IX: Magnetic moment in each magnetic phase of $YMnO_3$.

Atom No.	Position	A_1	A_2	B_1	B_2
1	(x,0,z)	(0,m,0)	(m,0,0)	(m,0,0)	(0,m,0)
2	(0,x,z)	(-$\sqrt{3}m$/2,-m/2,0)	(-m/2,$\sqrt{3}m$/2,0)	(-m/2,$\sqrt{3}m$/2,z)	(-$\sqrt{3}m$/2,-m/2,0)
3	(1-x, 1-x, z)	($\sqrt{3}m$/2,-m/2,0)	(-m/2,-$\sqrt{3}m$/2,0)	(-m/2,-$\sqrt{3}m$/2,z)	($\sqrt{3}m$/2,-m/2,0)
4	(1-x, 0, 0.5+z)	(0,-m,0)	(-m,0,0)	(m,0,0)	(0,m,0)
5	(0, 1-x, 0.5+z)	($\sqrt{3}m$/2,m/2,0)	(m/2,-$\sqrt{3}m$/2,0)	(-m/2,$\sqrt{3}m$/2,z)	(-$\sqrt{3}m$/2,-m/2,0)
6	(x, x, 0.5+z)	(-$\sqrt{3}m$/2,m/2,0)	(m/2,$\sqrt{3}m$/2,0)	(-m/2,-$\sqrt{3}m$/2,z)	($\sqrt{3}m$/2,-m/2,0)

Table X shows the symmetries and classification of SHG A_1, A_2, B_1 and B_2 phases. The in-plane even SHG elements $\chi_{abc}^{\text{even}}(a, b, c \in \{x, y\})$ vanish in all magnetic phase, because $G_0 = 6mm$ has out-of-plane C_2 symmetry. However, the isomorphic group G_1 of B_1 and B_2 phases break the in-plane C_2 symmetry, leading to the nonzero of in-plane odd SHG, as shown in Table X. Besides, the symmetry of A_2 phase (MPG: $6m'm'$) allows the LMO effect. Despite the same crystal structure, different magnetic structures lead to distinctive SHG and LMO features.

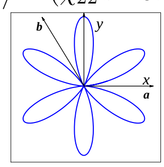
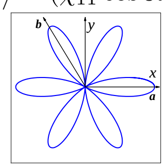
Suppl. Note 5.4. Role of spin-orbit coupling effect

From the above analysis, we can see that magnetic groups affect the classification of SHG. In addition, spin-orbit coupling(SOC) plays a crucial role in the symmetry of magnetic materials [32]. The stronger SOC always



Supplementary Figure 5: Band structures of $YMnO_3$. (a) A_1, (b) A_2, (c) B_1 and (d) B_2 phase, respectively.

Suppl. Tab. X: Characters of SHG and LMO effects of $RMnO_3$ with different magnetic structures.

Magnetic phase	**MSG**	**SHG type and nonzero odd SHG elements**	**In plane $I_{//}$ SHG**	**LMO**
A_1	$P6_3cm$	O-woP, $G_1 = 6mm$ $\chi^{\text{odd}}_{xxz} = \chi^{\text{odd}}_{xzx} = \chi^{\text{odd}}_{yyz} = \chi^{\text{odd}}_{yzy}$ $\chi^{\text{odd}}_{zxx} = \chi^{\text{odd}}_{zyy}, \chi^{\text{odd}}_{zzz}$	×	×
A_2	$P6_3c'm'$	BW-woP, $G_1 = 622$ $\chi^{\text{odd}}_{xyz} = \chi^{\text{odd}}_{xzy} = -\chi^{\text{odd}}_{yxz} = -\chi^{\text{odd}}_{yzx}$	×	✓
B_1	$P6_3'cm'$	BW-woP, $G_1 = \bar{6}m2$ $\chi^{\text{odd}}_{yyy} = -\chi^{\text{odd}}_{yxx} = -\chi^{\text{odd}}_{xyx} = -\chi^{\text{odd}}_{xxy}$	$I_{//} = (\chi_{22} \sin 3\theta)^2$ 	×
B_2	$P6_3'c'm$	BW-woP, $G_1 = \bar{6}2m$ $\chi^{\text{odd}}_{xxx} = -\chi^{\text{odd}}_{xyy} = -\chi^{\text{odd}}_{yxy} = -\chi^{\text{odd}}_{yyx}$	$I_{//} = (\chi_{11} \cos 3\theta)^2$ 	×

1. The coordinate systems of the above four phases are the same, i.e., $\mathbf{a} = \mathbf{x}$, $\mathbf{b} = -\mathbf{x}/2 + \sqrt{3}\mathbf{y}/2$
2. The even parts of SHG of each magnetic structure are the same, and χ^{even}_{ijk} is constrained by G_0=$6mm$, i.e. $\chi^{\text{even}}_{xxz} = \chi^{\text{even}}_{xzx} = \chi^{\text{even}}_{yyz} = \chi^{\text{even}}_{yzy}$, $\chi^{\text{even}}_{zxx} = \chi^{\text{even}}_{zyy}$, χ^{even}_{zzz}.

results in more evident SHG effect (see the examples of monolayer VSe_2 and Fe_3GeTe_2 in Supplementary Note 5 Suppl. Note 5.2), while the disappearance of the SOC effect leads to the vanish of SHG effect contributed by magnetism (see Supplementary Note 5 Suppl. Note 5.1). This can be understood as follows. In coplanar magnetic materials without SOC, the spin rotation symmetry (operator R_S) also retains. Even though T is broken, a combination symmetry R_ST is preserved in these systems [33], and R_ST acts as "effective T symmetry" [34] for SHG susceptibilities. No SHG effect can be observed in coplanar magnetic materials without SOC if the parent phases have inversion symmetry, such as the O-wP, G-wP, PT-wP, and BW-wP types of SHG. This is similar to that of the bulk photovoltaic effect in coplanar magnetic materials [35, 36]. While for the coplanar magnetic materials with broken inversion symmetry in parent phases and without SOC, the odd parts of O-woP, G-woP, and BW-woP types of SHG vanish as these types of SHG are only induced by magnetism. In contrast, the even parts of SHG still exist due to the contribution from crystal asymmetry.

Suppl. Note 5.5. The characteristics of zero frequency limit of χ^{even} and χ^{odd}

The other characteristic is that odd SHG susceptibilities vanish at the zero frequency limit ($\omega \to 0$) [3], while the even parts can be nonzero for semiconducting magnetic materials. The even part of SHG ($\chi^{\text{even}} = \operatorname{Re}\chi^{\text{even}} + \operatorname{Im}\chi^{\text{even}}$) takes the form of $\int \frac{\operatorname{Re} A}{\omega_{mn}-\eta\omega-i/\tau} d[\mathbf{k}]$ and the odd part ($\chi^{\text{odd}} = \operatorname{Re}\chi^{\text{odd}} + \operatorname{Im}\chi^{\text{odd}}$) adopts the form of $\int \frac{\operatorname{Im} A}{\omega_{mn}-\eta\omega-i/\tau} d[\mathbf{k}]$, according to Eq. (S5) and hereafter discussion. In the static limit $\omega \to 0$, SHG coefficient is pure real, so $\operatorname{Im}\chi^{\text{even}}$ and $\operatorname{Im}\chi^{\text{odd}}$ vanish. Therefore, the odd parts are zero [3], while the even parts of SHG can survive, because $\operatorname{Re}\chi^{\text{even}}$ and $\operatorname{Re}\chi^{\text{odd}}$ have the forms of $\int \operatorname{Re} A \operatorname{Re}\left(\frac{1}{\omega_{mn}-\eta\omega-i/\tau}\right) d[\mathbf{k}]$ and $\int \operatorname{Im} A \operatorname{Im}\left(\frac{1}{\omega_{mn}-\eta\omega-i/\tau}\right) d[\mathbf{k}]$, respectively. $\operatorname{Im}\left(\frac{1}{\omega_{mn}-\eta\omega-i/\tau}\right)$ is zero at static limits, while $\operatorname{Re}\left(\frac{1}{\omega_{mn}-\eta\omega-i/\tau}\right)$ is nonzero when $\omega = 0$. The calculated static limits of SHG of monolayer VSe_2 in Figure 4(c) and Figure 3(c,f) are consistent with the above analysis, similar to calculated results of bilayer CrI_3 [3, 22].

Supplementary Note 6. SHG AND LMO EFFECTS MATERIALS DATABASE

Suppl. Tab. XI: Clarifications of SHG and LMO effects in MAGNDATA database. BCS-ID: 0.1-0.835, 1.0.1-1.0.52, 1.1-1.663, 2.1-2.86, and 3.1-3.19. The underline wave symbols mean the materials have appeared in front of this table. The meaning of the SHG type see Table II in the main text, the symmetries of SHG and LMO effect refer to Supplementary Note 3 and Table II, respectively. The following table can also be found in the home-made website "Classification of SHG effect in magnetic materials".

BCS-ID	Formula	Parent SG	MSG	MPG	SHG	LMO
0.1	$LaMnO_3$	$Pnma$ (62)	$Pn'ma'$ (62.448)	$m'm'm$	×	✓
0.2	$Cd_2Os_2O_7$	$Fd\bar{3}m$ (227)	$Fd\bar{3}m'$ (227.131)	$m\bar{3}m'$	×	×
0.3	Ca_3LiOsO_6	$R\bar{3}c$ (167)	$C2'/c'$ (15.89)	$2'/m'$	×	✓
0.4	$NiCr_2O_4$	$I4_1/amd$ (141)	$Fd'd'd$ (70.530)	$m'm'm$	×	✓
0.5	Cr_2S_3	$R\bar{3}$ (148)	$P\bar{1}$ (2.4)	$\bar{1}$	×	✓
0.6	$YMnO_3$	$P6_3cm$ (185)	$P6_3cm$ (185.197)	$6mm$	O-woP	×
0.7	$ScMnO_3$	$P6_3cm$ (185)	$P6_3c'm'$ (185.201)	$6m'm'$	BW-woP	✓
0.8	$ScMnO_3$	$P6_3cm$ (185)	$P6_3$ (173.129)	6	O-woP	✓
0.9	GdB_4	$P4/mbm$ (127)	$P4/m'b'm'$ (127.395)	$4/m'm'm'$	PT-wP	×
0.10	$DyFeO_3$	$Pnma$ (62)	$P2_12_12_1$ (19.25)	222	O-wP	×
0.11	$DyFeO_3$	$Pnma$ (62)	$Pn'a'2_1$ (33.148)	$m'm'2$	BW-wP	✓
0.12	$U_3Ru_4Al_{12}$	$P6_3/mmc$ (194)	$Cmcm'$ (63.461)	$m'mm$	PT-wP	×
0.13	$Ca_3Co_{2-x}Mn_xO_6$	$R\bar{3}c$ (167)	$R3c$ (161.69)	$3m$	O-wP	×
0.14	Gd_5Ge_4	$Pnma$ (62)	$Pnm'a$ (62.444)	$m'mm$	PT-wP	×
0.15	MnF_2	$P4_2/mnm$ (136)	$P4_2'/mnm'$ (136.499)	$4'/mm'm$	×	×
0.16	$EuTiO_3$	$I4/mcm$ (140)	$Fm'mm$ (69.523)	$m'mm$	PT-wP	×
0.17	$FePO_4$	$Pnma$ (62)	$P2_12_12_1$ (19.25)	222	O-wP	×
0.18	$BaMn_2As_2$	$I4/mmm$ (139)	$I4'/m'm'm$ (139.536)	$4'/m'm'm$	PT-wP	×
0.19	$MnTiO_3$	$R\bar{3}$ (148)	$R\bar{3}'$ (148.19)	$\bar{3}'$	PT-wP	×
0.20	$MnTe_2$	$Pa\bar{3}$ (205)	$Pa\bar{3}$ (205.33)	$m\bar{3}$	×	×
0.21	$PbNiO_3$	$R3c$ (161)	$R3c$ (161.69)	$3m$	O-woP	×
0.22	DyB_4	$P4/mbm$ (127)	$Pb'am$ (55.355)	$m'mm$	PT-wP	×
0.23	$Ca_3Mn_2O_7$	$Cmc2_1$ (36)	$Cm'c2_1'$ (36.174)	$m'm2'$	BW-woP	✓
0.24	$LiMnPO_4$	$Pnma$ (62)	$Pn'm'a'$ (62.449)	$m'm'm'$	PT-wP	×
0.25	$NaOsO_3$	$Pnma$ (62)	$Pn'ma'$ (62.448)	$m'm'm$	×	✓
0.26	TmAgGe	$P\bar{6}2m$ (189)	$Am'm'2$ (38.191)	$m'm'2$	BW-woP	✓
0.27	YFe_4Ge_2	$Pnnm$ (58)	$Pn'n'm'$ (58.399)	$m'm'm'$	PT-wP	×
0.28	$LiFeSi_2O_6$	$P2_1/c$ (14)	$P2_1/c'$ (14.78)	$2/m'$	PT-wP	×
0.29	$Er_2Ti_2O_7$	$Fd\bar{3}m$ (227)	$I4_1'/am'd$ (141.554)	$4'/mm'm$	×	×
0.30	$YbMnO_3$	$P6_3cm$ (185)	$P6_3'c'm$ (185.199)	$6'mm'$	BW-woP	×
0.31	$HoMnO_3$	$P6_3cm$ (185)	$P6_3c'm'$ (185.201)	$6m'm'$	BW-woP	✓
0.32	$HoMnO_3$	$P6_3cm$ (185)	$P6_3cm$ (185.197)	$6mm$	O-woP	×
0.33	$\utilde{HoMnO_3}$	$P6_3cm$ (185)	$P6_3cm$ (185.197)	$6mm$	O-woP	×
0.34	$La_{0.5}Sr_{0.5}FeO_{2.5}F_{0.5}$	$Pnma$ (062)	$Pn'ma'$ (62.448)	$m'm'm$	×	✓
0.35	Cu_2OSeO_3	$P2_13$ (198)	$R3$ (146.10)	3	O-woP	✓
0.36	NiF_2	$P4_2/mnm$ (136)	$Pnn'm'$ (58.398)	$m'm'm$	×	✓
0.37	$U_3Al_2Si_3$	$I4$ (79)	$C2'$ (5.15)	$2'$	BW-woP	✓
0.38	$GaFeO_3$	$Pna2_1$ (33)	$Pna'2_1'$ (33.147)	$m'm2'$	BW-woP	✓
0.39	Nd_2NaRuO_6	$P2_1/n$ (14)	$P2_1/c$ (14.75)	$2/m$	×	✓
0.40	Mn_2O_3-alpha	$Pbca$ (61)	$Pbca$ (61.433)	mmm	×	×
0.41	$\utilde{Mn_2O_3\text{-alpha}}$	$Pbca$ (61)	$Pbca$ (61.433)	mmm	×	×
0.42	$HoMnO_3$	$P6_3cm$ (185)	$P6_3'c'm$ (185.199)	$6'mm'$	BW-woP	×
0.43	$HoMnO_3$	$P6_3cm$ (185)	$P6_3'cm'$ (185.2)	$6'mm'$	BW-woP	×
0.44	$YMnO_3$	$P6_3cm$ (185)	$P6_3'$ (173.131)	$6'$	BW-woP	×

Continued on next page

Suppl. Tab. XI – continued from previous page

BCS-ID	Formula	Parent	MSG	MPG	SHG type	LMO
0.45	La_2NiO_4	$P4_2/ncm$ (138)	$Pc'c'n$ (56.369)	$m'm'm$	×	✓
0.46	$CaBaCo_4O_7$	$Pbn2_1$ (33)	$Pna'2_1'$ (33.147)	$m'm2'$	BW-woP	✓
0.47	$Gd_2Sn_2O_7$	$Fd\bar{3}m$ (227)	$I4_1'/amd'$ (141.555)	$4'/mm'm$	×	×
0.48	$Tb_2Sn_2O_7$	$Fd\bar{3}m$ (227)	$I4_1/am'd'$ (141.557)	$4/mm'm'$	×	✓
0.49	$Ho_2Ru_2O_7$	$Fd\bar{3}m$ (227)	$I4_1/am'd'$ (141.557)	$4/mm'm'$	×	✓
0.50	$MnTiO_3$	$R3c$ (161)	Cc' (9.39)	m'	BW-woP	✓
0.51	$Ho_2Ru_2O_7$	$Fd\bar{3}m$ (227)	$I4_1/am'd'$ (141.557)	$4/mm'm'$	×	✓
0.52	$K_yFe_{2-x}Se_2$	$I4/m$ (87)	$C2'/m'$ (12.62)	$2'/m'$	×	✓
0.53	$Rb_yFe_{2-x}Se_2$	$I4/m$ (87)	$C2'/m'$ (12.62)	$2'/m'$	×	✓
0.54	$Rb_yFe_{2-x}Se_2$	$I4/m$ (87)	$I4/m'$ (87.78)	$4/m'$	PT-wP	×
0.55	K_yFe_2-xSe_2	$I4/m$ (87)	$I4/m'$ (87.78)	$4/m'$	PT-wP	×
0.56	$Ba_2CoGe_2O_7$	$P\bar{4}2_1m$ (113)	$Cm'm2'$ (35.167)	$m'm2'$	BW-woP	✓
0.57	$ScFeO_3$	$R3c$ (161)	Cc' (9.39)	m'	BW-woP	✓
0.58	$CoAl_2O_4$	$Fd\bar{3}m$ (227)	$I4_1'/a'm'd$ (141.556)	$4'/m'm'm$	PT-wP	×
0.59	Cr_2O_3	$R\bar{3}c$ (167)	$R\bar{3}'c'$ (167.106)	$\bar{3}'m'$	PT-wP	×
0.60	$[NH_2(CH_3)_2]_n[Fe^{III}Fe^{II}(HCOO)_6]_n$	$R\bar{3}c$ (167)	$R\bar{3}c'$ (167.107)	$\bar{3}m'$	×	✓
0.61	$Li_2FeP_2O_7$	$P2_1/c$ (14)	$P2_1/c$ (14.75)	$2/m$	×	✓
0.62	$SrMn_2V_2O_8$	$I4_1cd$ (110)	$Ib'a2'$ (45.237)	$m'm2'$	BW-woP	✓
0.63	Ho_2CrSbO_7	$Fd\bar{3}m$ (227)	$I4_1/am'd'$ (141.557)	$4/mm'm'$	×	✓
0.64	MnV_2O_4	$I4_1/a$ (88)	$I4_1/a$ (88.81)	$4/m$	×	✓
0.65	Fe_2O_3-alpha	$R\bar{3}c$ (167)	$C2'/c'$ (15.89)	$2'/m'$	×	✓
0.66	Fe_2O_3-alpha	$R\bar{3}c$ (167)	$P\bar{1}$ (2.4)	$\bar{1}$	×	✓
0.67	$BiFe_{0.5}Sc_{0.5}O_3$	$Ima2$ (46)	$Im'a2'$ (46.243)	$m'm2'$	BW-woP	✓
0.68	$BiFe_{0.5}Sc_{0.5}O_3$	$Pnma$ (62)	$Pn'm'a$ (62.446)	$m'm'm$	×	✓
0.69	$Co_4(OH)_2(C_{10}H_{16}O_4)_3$	$P2_1/c$ (14)	$P2_1'/c'$ (14.79)	$2'/m'$	×	✓
0.70	$Na_3Co(CO_3)_2Cl$	$Fd\bar{3}$ (203)	$Fd\bar{3}$ (203.26)	$m\bar{3}$	×	×
0.71	$Li_2Ni(SO_4)_2$	$Pbca$ (61)	$Pb'c'a'$ (61.437)	$m'm'm'$	PT-wP	×
0.72	$CaMnBi_2$	$P4/nmm$ (129)	$P4'/n'm'm$ (129.416)	$4'/m'm'm$	PT-wP	×
0.73	$SrMnBi_2$	$I4/mmm$ (139)	$I4'/m'm'm$ (139.536)	$4'/m'm'm$	PT-wP	×
0.74	$Mn_3Cu_{0.5}Ge_{0.5}N$	$Pm\bar{3}m$ (221)	$R\bar{3}m$ (166.97)	$\bar{3}m$	×	×
0.75	Cr_2WO_6	$P4_2/mnm$ (136)	$Pn'nm$ (58.395)	$m'mm$	PT-wP	×
0.76	Cr_2TeO_6	$P4_2/mnm$ (136)	$Pn'nm$ (58.395)	$m'mm$	PT-wP	×
0.77	$Tb_2Ti_2O_7$	$Fd\bar{3}m$ (227)	$R\bar{3}m'$ (166.101)	$\bar{3}m'$	×	✓
0.78	NiN_2O_6	$R\bar{3}$ (148)	$R\bar{3}$ (148.17)	$\bar{3}$	×	✓
0.79	$CaIrO_3$	$Cmcm$ (63)	$Cm'cm'$ (63.464)	$m'm'm$	×	✓
0.80	U_2Pd_2In	$P4/mbm$ (127)	$P4'/m'bm'$ (127.394)	$4'/m'm'm$	PT-wP	×
0.81	U_2Pd_2Sn	$P4/mbm$ (127)	$P4'/m'bm'$ (127.394)	$4'/m'm'm$	PT-wP	×
0.82	Gd_2CuO_4	$Aeam$ (64)	$Cm'ca'$ (64.476)	$m'm'm$	×	✓
0.83	$LiFeP_2O_7$	$P2_1$ (4)	$P2_1$ (4.7)	2	O-woP	✓
0.84	Mn_2FeMoO_6	$R3$ (146)	$R3$ (146.10)	3	O-woP	✓
0.85	$KCo_4(PO_4)_3$	$Pnnm$ (58)	$Pnn'm'$ (58.398)	$m'm'm$	×	✓
0.86	$KMn_4(PO_4)_3$	$Pnam$ (62)	$Pnma'$ (62.445)	$m'mm$	PT-wP	×
0.87	$NaFePO_4$	$Pnma$ (62)	$Pnma'$ (62.445)	$m'mm$	PT-wP	×
0.88	$LiNiPO_4$	$Pnma$ (62)	$Pnm'a$ (62.444)	$m'mm$	PT-wP	×
0.89	$BaMn_2Bi_2$	$I4/mmm$ (139)	$I4'/m'm'm$ (139.536)	$4'/m'm'm$	PT-wP	×
0.90	$Rb_2Fe_2O(AsO_4)_2$	$Pnma$ (62)	$Pnma$ (62.441)	mmm	×	×
0.91	$Rb_2Fe_2O(AsO_4)_2$	$Pnma$ (62)	$Pn'ma'$ (62.448)	$m'm'm$	×	✓
0.92	$CaMn_2Sb_2$	$P\bar{3}m1$ (164)	$C2'/m$ (12.60)	$2'/m$	PT-wP	×
0.93	$Ca_2Fe_2O_5$	$Pcmn$ (62)	$Pcm'n'$ (62.446)	$m'm'm$	×	✓
0.94	$TeNiO_3$	$Pnma$ (62)	$Pn'm'a$ (62.446)	$m'm'm$	×	✓
0.95	$LiFePO_4$	$Pnma$ (62)	$Pnma'$ (62.445)	$m'mm$	PT-wP	×

Continued on next page

Suppl. Tab. XI – continued from previous page

BCS-ID	Formula	Parent	MSG	MPG	SHG type	LMO
0.96	$CoSO_4$	$Pnma$ (62)	$Pnma$ (62.441)	mmm	×	×
0.97	$FeSb_2O_4$	$P4_2/mbc$ (135)	$Pmc2_1$ (26.66)	$mm2$	O-wP	×
0.98	$YBaMn_2O_{5.5}$	$Icam$ (72)	$Ib'a'm$ (72.543)	$m'm'm$	×	✓
0.99	$YBaMn_2O_{5.5}$	$Icam$ (72)	$C2/m$ (12.58)	$2/m$	×	✓
0.100	$YCr_{0.5}Mn_{0.5}O_3$	$Pnma$ (62)	$Pn'ma'$ (62.448)	$m'm'm$	×	✓
0.101	Mn_2GeO_4	$Pnma$ (62)	$Pn'm'a$ (62.446)	$m'm'm$	×	✓
0.102	Mn_2GeO_4	$Pnma$ (62)	$Pnma$ (62.441)	mmm	×	×
0.103	Mn_2GeO_4	$Pnma$ (62)	$P2_1/c$ (14.75)	$2/m$	×	✓
0.104	$ErVO_3$	$Pbnm$ (62)	$P2_1'/m'$ (11.54)	$2'/m'$	×	✓
0.105	$ErVO_3$	$Pbnm$ (62)	$P2_1/c$ (14.75)	$2/m$	×	✓
0.106	$DyVO_3$	$Pbnm$ (62)	$P2_1'/m'$ (11.54)	$2'/m'$	×	✓
0.107	$Ho_2Ge_2O_7$	$P4_12_12$ (92)	$P4_12_12$ (92.111)	422	O-woP	×
0.108	Mn_3Ir	$Pm\bar{3}m$ (221)	$R\bar{3}m'$ (166.101)	$\bar{3}m'$	×	✓
0.109	Mn_3Pt	$Pm\bar{3}m$ (221)	$R\bar{3}m'$ (166.101)	$\bar{3}m'$	×	✓
0.110	Cr_2O_3	$R\bar{3}c$ (167)	$C2'/c$ (15.87)	$2'/m$	PT-wP	×
0.111	$Co_4Nb_2O_9$	$P\bar{3}c1$ (165)	$P\bar{3}'c'1$ (165.94)	$\bar{3}'m'$	PT-wP	×
0.112	$FeBO_3$	$R\bar{3}c$ (167)	$C2'/c'$ (15.89)	$2'/m'$	×	✓
0.113	$NiCO_3$	$R\bar{3}c$ (167)	$C2/c$ (15.85)	$2/m$	×	✓
0.114	$CoCO_3$	$R\bar{3}c$ (167)	$C2/c$ (15.85)	$2/m$	×	✓
0.115	$MnCO_3$	$R\bar{3}c$ (167)	$C2/c$ (15.85)	$2/m$	×	✓
0.116	$FeCO_3$	$R\bar{3}c$ (167)	$R\bar{3}c$ (167.103)	$\bar{3}m$	×	×
0.117	$LuFeO_3$	$P6_3cm$ (185)	$P6_3c'm'$ (185.201)	$6m'm'$	BW-woP	✓
0.118	$Ba_5Co_5ClO_{13}$	$P6_3/mmc$ (194)	$P6_3'/m'm'c$ (194.268)	$6'/m'mm'$	×	×
0.119	$CoSe_2O_5$	$Pbcn$ (60)	$Pb'cn$ (60.419)	$m'mm$	PT-wP	×
0.120	$LiFe(SO_4)_2$	$P2_1/c$ (14)	$P2_1/c$ (14.75)	$2/m$	×	✓
0.121	$Li_2Co(SO_4)_2$	$P2_1/c$ (14)	$P2_1'/c'$ (14.79)	$2'/m'$	×	✓
0.122	$Li_2Mn(SO_4)_2$	$P2_1/c$ (14)	$P2_1/c$ (14.75)	$2/m$	×	✓
0.123	Mn_3NiN	$Pm\bar{3}m$ (221)	$R\bar{3}$ (148.17)	$\bar{3}$	×	✓
0.124	Mn_3NiN	$Pm\bar{3}m$ (221)	$R\bar{3}$ (148.17)	$\bar{3}$	×	✓
0.125	$MnGeO_3$	$R\bar{3}$ (148)	$R\bar{3}'$ (148.19)	$\bar{3}'$	PT-wP	×
0.126	$NpCo_2$	$Fd\bar{3}m$ (227)	$I4_1'/a'm'd$ (141.556)	$4'/m'm'm$	PT-wP	×
0.127	$Dy_3Al_5O_{12}$	$Ia\bar{3}d$ (230)	$Ia\bar{3}d'$ (230.148)	$m\bar{3}m'$	×	×
0.128	$FeSO_4F$	$C2/c$ (15)	$C2'/c'$ (15.89)	$2'/m'$	×	✓
0.129	$Cu_3Mo_2O_9$	$Pnma$ (62)	$P2_1'2_1'2_1$ (19.27)	$2'2'2$	BW-wP	✓
0.130	$Cu_3Mo_2O_9$	$Pnma$ (62)	$Pm'c2_1'$ (26.68)	$m'm2'$	BW-wP	✓
0.131	$Mn(N(CN_2))_2$	$Pnnm$ (58)	$Pnn'm'$ (58.398)	$m'm'm$	×	✓
0.132	$Fe(N(CN_2))_2$	$Pnnm$ (58)	$Pnn'm'$ (58.398)	$m'm'm$	×	✓
0.133	$Ni_3B_7O_{13}Cl$	$Pca2_1$ (29)	$Pc'a2_1'$ (29.101)	$m'm2'$	BW-woP	✓
0.134	$Mn_3B_7O_{13}I$	$Pca2_1$ (29)	$Pc'a2_1'$ (29.101)	$m'm2'$	BW-woP	✓
0.135	$Ni_3B_7O_{13}Br$	$Pca2_1$ (29)	$Pc'a2_1'$ (29.101)	$m'm2'$	BW-woP	✓
0.136	$Co_3B_7O_{13}Br$	$Pca2_1$ (29)	$Pc'a2_1'$ (29.101)	$m'm2'$	BW-woP	✓
0.137	$Cu_2V_2O_7$	$Fdd2$ (43)	$Fd'd'2$ (43.227)	$m'm'2$	BW-woP	✓
0.138	$BiCrO_3$	$C2/c$ (15)	$C2/c$ (15.85)	$2/m$	×	✓
0.139	$BiCrO_3$	$C2/c$ (15)	$P\bar{1}$ (2.4)	$\bar{1}$	×	✓
0.140	$LuFe_4Ge_2$	$P4_2/mnm$ (136)	$Pn'n'm'$ (58.399)	$m'm'm'$	PT-wP	×
0.141	Tb_5Ge_4	$Pnma$ (62)	$Pnm'a$ (62.444)	$m'mm$	PT-wP	×
0.142	Fe_2TeO_6	$P4_2/mnm$ (136)	$P4_2/m'n'm'$ (136.503)	$4/m'm'm'$	PT-wP	×
0.143	Cr_2TeO_6	$P4_2/mnm$ (136)	$Pn'nm$ (58.395)	$m'mm$	PT-wP	×
0.144	Cr_2WO_6	$P4_2/mnm$ (136)	$Pn'nm$ (58.395)	$m'mm$	PT-wP	×
0.145	Co_3TeO_6	$C2/c$ (15)	$C2'/c$ (15.87)	$2'/m$	PT-wP	×
0.146	$EuZrO_3$	$Pnma$ (62)	$Pnm'a$ (62.444)	$m'mm$	PT-wP	×

Continued on next page

Suppl. Tab. XI – continued from previous page

BCS-ID	Formula	Parent	MSG	MPG	SHG type	LMO
0.147	$EuZrO_3$	$Pnma$ (62)	$Pn'm'a'$ (62.449)	$m'm'm'$	PT-wP	×
0.148	La_2LiRuO_6	$P2_1/n$ (14)	$P2_1/c$ (14.75)	$2/m$	×	✓
0.149	$Nd_3Ru_4Al_{12}$	$P6_3/mmc$ (194)	$Cm'c'm$ (63.462)	$m'm'm$	×	✓
0.15	NiS_2	$Pa\bar{3}$ (205)	$Pa\bar{3}$ (205.33)	$m\bar{3}$	×	×
0.151	$Tm_2Mn_2O_7$	$Fd\bar{3}m$ (227)	$I4_1/am'd'$ (141.557)	$4/mm'm'$	×	✓
0.152	$LiFePO_4$	$Pnma$ (62)	$P2_1/c'$ (14.78)	$2/m'$	PT-wP	×
0.153	Bi_2RuMnO_7	$Fd\bar{3}m$ (227)	$Fd'd'd$ (70.530)	$m'm'm$	×	✓
0.154	$Er_2Ru_2O_7$	$Fd\bar{3}m$ (227)	$I4_1'/am'd$ (141.554)	$4'/mm'm$	×	×
0.155	$CaMnGe_2O_6$	$C2/c$ (15)	$P\bar{1}'$ (2.6)	$\bar{1}'$	PT-wP	×
0.156	$CaMnGe_2O_6$	$C2/c$ (15)	$C2'/c$ (15.87)	$2'/m$	PT-wP	×
0.157	$Yb_2Sn_2O_7$	$Fd\bar{3}m$ (227)	$I4_1/am'd'$ (141.557)	$4/mm'm'$	×	✓
0.158	$Yb_2Ti_2O_7$	$Fd\bar{3}m$ (227)	$I4_1/am'd'$ (141.557)	$4/mm'm'$	×	✓
0.159	$DyCoO_3$	$Pbnm$ (62)	$Pn'm'a'$ (62.449)	$m'm'm'$	PT-wP	×
0.160	$TbCoO_3$	$Pbnm$ (62)	$Pnm'a$ (62.444)	$m'mm$	PT-wP	×
0.161	$CoSe_2O_5$	$Pbcn$ (60)	$Pb'cn$ (60.419)	$m'mm$	PT-wP	×
0.162	$NdCrTiO_5$	$Pbam$ (55)	$Pbam'$ (55.356)	$m'mm$	PT-wP	×
0.163	$MnPS_3$	$C2/m$ (12)	$C2'/m$ (12.60)	$2'/m$	PT-wP	×
0.164	Y_2MnCoO_6	$P2_1/c$ (14)	$P2_1'/c'$ (14.79)	$2'/m'$	×	✓
0.165	$SrMn(VO_4)(OH)$	$P2_12_12_1$ (19)	$P2_1$ (4.7)	2	O-woP	✓
0.166	Ce_2PdGe_3	$P4_2/mmc$ (131)	$P4_2'/m'm'c$ (131.440)	$4'/m'm'm$	PT-wP	×
0.167	$Nd_3Sb_3Mg_2O_{14}$	$R\bar{3}m$ (166)	$R\bar{3}m'$ (166.101)	$\bar{3}m'$	×	✓
0.168	$NH_4Fe_2F_6$	$Pnma$ (62)	$Pnma$ (62.441)	mmm	×	×
0.169	U_3As_4	$I\bar{4}3d$ (220)	$R3c'$ (161.71)	$3m'$	BW-woP	✓
0.170	U_3P_4	$I\bar{4}3d$ (220)	$R3c'$ (161.71)	$3m'$	BW-woP	✓
0.171	$DyScO_3$	$Pnma$ (62)	$Pn'm'a'$ (62.449)	$m'm'm'$	PT-wP	×
0.172	$Y_3Co_{3.25}Al_{0.75}$	$Cmcm$ (63)	$Cm'cm'$ (63.464)	$m'm'm$	×	✓
0.173	$Pr_3Ru_4Al_{12}$	$P6_3/mmc$ (194)	$Cm'c'm$ (63.462)	$m'm'm$	×	✓
0.174	$Pr_3Ru_4Al_{12}$	$P6_3/mmc$ (194)	$C2'/c'$ (15.89)	$2'/m'$	×	✓
0.175	$Ca_2CoSi_2O_7$	$P\bar{4}2_1m$ (113)	$P2_12_1'2'$ (18.19)	$2'2'2$	BW-woP	✓
0.176	$Mn_3Ti_2Te_6$	$P\bar{3}1c$ (163)	$C2'/c'$ (15.89)	$2'/m'$	×	✓
0.177	Mn_3GaN	$Pm\bar{3}m$ (221)	$R\bar{3}m$ (166.97)	$\bar{3}m$	×	×
0.178	CoF_2	$P4_2/mnm$ (136)	$P4_2'/mnm'$ (136.499)	$4'/mm'm$	×	×
0.179	$FeCl_5D_2O(ND_4)_2$	$P2_1/c$ (14)	$P2_1'$ (4.9)	$2'$	BW-wP	✓
0.180	$MnPSe_3$	$R\bar{3}$ (148)	$P\bar{1}'$ (2.6)	$\bar{1}'$	PT-wP	×
0.181	$Nd_{15}Ge_9C_{0.39}$	$P6_3mc$ (186)	$P6_3m'c'$ (186.207)	$6m'm'$	BW-woP	✓
0.182	$KCrF_4$	$Pnma$ (62)	$Pn'ma$ (62.443)	$m'mm$	PT-wP	×
0.183	$KMnFeF_6$	$P4_2bc$ (106)	$Pb'a2'$ (32.137)	$m'm2'$	BW-woP	✓
0.184	Nd_5Si_4	$P4_12_12$ (92)	$P4_12_1'2'$ (92.114)	$42'2'$	BW-woP	✓
0.185	Nd_5Ge_4	$Pnma$ (62)	$Pnm'a'$ (62.447)	$m'm'm$	×	✓
0.186	$CeMnAsO$	$P4/nmm$ (129)	$P4'/n'm'm$ (129.416)	$4'/m'm'm$	PT-wP	×
0.187	$CeMnAsO$	$P4/nmm$ (129)	$Pm'mn$ (59.407)	$m'mm$	PT-wP	×
0.188	$CeMnAsO$	$P4/nmm$ (129)	$P2'/c$ (13.67)	$2'/m$	PT-wP	×
0.189	$CeMn_2Ge_4O_{12}$	$P4/nbm$ (125)	$P4'/nbm'$ (125.367)	$4'/mm'm$	×	×
0.190	$CeMnCoGe_4O_{12}$	$P4/nbm$ (125)	$Pb'an'$ (50.282)	$m'm'm$	×	✓
0.191	$BaCuF_4$	$Cmc2_1$ (36)	$Cm'c'2_1$ (36.176)	$m'm'2$	BW-woP	✓
0.192	$RbFe_2F_6$	$Pnma$ (62)	$Pnma$ (62.441)	mmm	×	×
0.193	$LiCoPO_4$	$Pnma$ (62)	$Pnma'$ (62.445)	$m'mm$	PT-wP	×
0.194	UPt_2Si_2	$P4/nmm$ (129)	$P4/n'm'm'$ (129.419)	$4/m'm'm'$	PT-wP	×
0.195	$Sr_2Ir_{0.92}Sn_{0.08}O_4$	$I4_1/acd$ (142)	$Ib'c'a$ (73.551)	$m'm'm$	×	✓
0.196	$Co_4Nb_2O_9$	$P\bar{3}c1$ (165)	$C2/c'$ (15.88)	$2/m'$	PT-wP	×
0.197	$Co_4Nb_2O_9$	$P\bar{3}c1$ (165)	$C2/c'$ (15.88)	$2/m'$	PT-wP	×

Continued on next page

Suppl. Tab. XI – continued from previous page

BCS-ID	Formula	Parent	MSG	MPG	SHG type	LMO
0.198	$GdVO_4$	$I4_1/amd$ (141)	$I4_1'/a'm'd$ (141.556)	$4'/m'm'm$	PT-wP	×
0.199	Mn_3Sn	$P6_3/mmc$ (194)	$Cmc'm'$ (63.463)	$m'm'm$	×	✓
0.200	Mn_3Sn	$P6_3/mmc$ (194)	$Cm'cm'$ (63.464)	$m'm'm$	×	✓
0.201	$Ca_2PrCr_2NbO_9$	$Pnma$ (62)	$Pn'm'a$ (62.446)	$m'm'm$	×	✓
0.202	$Ca_2PrCr_2TaO_9$	$Pnma$ (62)	$Pn'm'a$ (62.446)	$m'm'm$	×	✓
0.203	Mn_3Ge	$P6_3/mmc$ (194)	$C2'/m'$ (12.62)	$2'/m'$	×	✓
0.204	Ca_2MnReO_6	$P2_1/c$ (14)	$P2_1/c$ (14.75)	$2/m$	×	✓
0.205	Sr_2MnReO_6	$P2_1/c$ (14)	$P2_1'/c'$ (14.79)	$2'/m'$	×	✓
0.206	$Ca_2Fe_{0.885}Cr_{0.125}GaO_5$	$Pnma$ (62)	$Pn'm'a$ (62.446)	$m'm'm$	×	✓
0.207	$TlFe_{1.6}Se_2$	$I4/m$ (87)	$I4/m$ (87.75)	$4/m$	×	✓
0.208	$TlFe_{1.6}Se_2$	$I4/m$ (87)	$C2'/m$ (12.60)	$2'/m$	PT-wP	×
0.209	$TlFe_{1.6}Se_2$	$I4/m$ (87)	$I4/m'$ (87.78)	$4/m'$	PT-wP	×
0.210	Sr_2CoOsO_6	$B2/n$ (15)	$C2/c$ (15.85)	$2/m$	×	✓
0.211	Ca_2MnO_4	$I4_1/acd$ (142)	$I4_1'/a'cd'$ (142.568)	$4'/m'm'm$	PT-wP	×
0.212	$Sr_2Mn_3As_2O_2$	$I4/mmm$ (139)	$I4'/m'm'm$ (139.536)	$4'/m'm'm$	PT-wP	×
0.213	$Sr_2Mn_2CuAs_2O_2$	$I4/mmm$ (139)	$I4/mm'm'$ (139.537)	$4/mm'm'$	×	✓
0.214	$FePbBiO_4$	$P4_2/mbc$ (135)	$Pmc2_1$ (26.66)	$mm2$	O-wP	×
0.215	$BaNi_2P_2O_8$	$R\bar{3}$ (148)	$P\bar{1}'$ (2.6)	$\bar{1}'$	PT-wP	×
0.216	$SrEr_2O_4$	$Pnma$ (62)	$Pnma'$ (62.445)	$m'mm$	PT-wP	×
0.217	$LiCrGe_2O_6$	$P2_1/c$ (14)	$P2_1'/c$ (14.77)	$2'/m$	PT-wP	×
0.218	Co_2SiO_4	$Pnma$ (62)	$Pnma$ (62.441)	mmm	×	×
0.219	Co_2SiO_4	$Pnma$ (62)	$Pnma$ (62.441)	mmm	×	×
0.220	Mn_2SiO_4	$Pnma$ (62)	$Pn'm'a$ (62.446)	$m'm'm$	×	✓
0.221	Fe_2SiO_4	$Pnma$ (62)	$Pnma$ (62.441)	mmm	×	×
0.222	$CuMnAs$	$P4/nmm$ (129)	$Pm'mn$ (59.407)	$m'mm$	PT-wP	×
0.223	$Cu_{0.95}MnAs$	$Pnma$ (62)	$Pn'ma$ (62.443)	$m'mm$	PT-wP	×
0.224	$Nd_{0.5}Tb_{0.5}Co_2$	$Fd\bar{3}m$ (227)	$C2'/m'$ (12.62)	$2'/m'$	×	✓
0.225	$Nd_{0.5}Tb_{0.5}Co_2$	$Fd\bar{3}m$ (227)	$C2'/m'$ (12.62)	$2'/m'$	×	✓
0.226	$NdCo_2$	$Fd\bar{3}m$ (227)	$C2'/c'$ (15.89)	$2'/m'$	×	✓
0.227	$NdCo_2$	$Fd\bar{3}m$ (227)	$I4_1/am'd'$ (141.557)	$4/mm'm'$	×	✓
0.228	$TbCo_2$	$Fd\bar{3}m$ (227)	$R\bar{3}m'$ (166.101)	$\bar{3}m'$	×	✓
0.229	$Ba_2MnSi_2O_7$	$P\bar{4}2_1m$ (113)	$P\bar{4}2_1m$ (113.267)	$\bar{4}2m$	O-woP	×
0.230	$K_2CoP_2O_7$	$P4_2/mnm$ (136)	$Pn'nm$ (58.395)	$m'mm$	PT-wP	×
0.231	$TmMn_3O_6$	$Pmmn$ (59)	$Pmm'n'$ (59.410)	$m'm'm$	×	✓
0.232	$TmMn_3O_6$	$Pmmn$ (59)	$Pm'm'n$ (59.409)	$m'm'm$	×	✓
0.233	Mn_2FeSbO_6	$R\bar{3}$ (148)	$P\bar{1}$ (2.4)	$\bar{1}$	×	✓
0.234	$MnLaMnSbO_6$	$P4_2/n$ (86)	$P2'/c'$ (13.69)	$2'/m'$	×	✓
0.235	$MnPrMnSbO_6$	$P4_2/n$ (86)	$P42/n$ (86.67)	$4/m$	×	✓
0.236	$CaFe_4Al_8$	$I4/mmm$ (139)	$I4'/mmm'$ (139.535)	$4'/mm'm$	×	×
0.237	$Er_2Sn_2O_7$	$Fd\bar{3}m$ (227)	$I4_1'/amd'$ (141.555)	$4'/mm'm$	×	×
0.238	$Er_2Pt_2O_7$	$Fd\bar{3}m$ (227)	$I4_1'/amd'$ (141.555)	$4'/mm'm$	×	×
0.239	Ca_3LiRuO_6	$R\bar{3}c$ (167)	$C2'/c'$ (15.89)	$2'/m'$	×	✓
0.240	$Er_2Cu_2O_5$	$Pna2_1$ (33)	$Pna2_1$ (33.144)	$mm2$	O-woP	×
0.241	$Y_2Cu_2O_5$	$Pna2_1$ (33)	$Pna2_1$ (33.144)	$mm2$	O-woP	×
0.242	$Tm_2Cu_2O_5$	$Pna2_1$ (33)	$Pn'a'2_1$ (33.148)	$m'm'2$	BW-woP	✓
0.243	$Li_2Fe(SO_4)_2$	$Pbca$ (61)	$P2_1'/c$ (14.77)	$2'/m$	PT-wP	×
0.244	$Li_2Co(SO_4)_2$	$Pbca$ (61)	$Pb'c'a'$ (61.437)	$m'm'm'$	PT-wP	×
0.245	$Li_{1.5}Fe(SO_4)_2$	$Pbca$ (61)	$P2_1'/c$ (14.77)	$2'/m$	PT-wP	×
0.246	$LiFe(SO_4)_2$	$Pbca$ (61)	$Pb'c'a'$ (61.437)	$m'm'm'$	PT-wP	×
0.247	$Nd_2NiO_{4.11}$	$P4_2/ncm$ (138)	$P4_2/nc'm'$ (138.525)	$4/mm'm'$	×	✓
0.248	$TbPt_{0.8}Cu_{0.2}$	$Pnma$ (62)	$Pn'm'a$ (62.446)	$m'm'm$	×	✓

Continued on next page

Suppl. Tab. XI – continued from previous page

BCS-ID	Formula	Parent	MSG	MPG	SHG type	LMO
0.249	$NdNi_{0.6}Cu_{0.4}$	$Pnma$ (62)	$Pnm'a'$ (62.447)	$m'm'm$	×	✓
0.250	$(NH_2(CH_3)_2)(FeCo(HCOO)_6)$	$P\bar{3}c1$ (163)	$C2'/c'$ (15.89)	$2'/m'$	×	✓
0.251	$(NH_2(CH_3)_2)(FeMn(HCOO)_6)$	$P\bar{3}c1$ (163)	$C2'/c'$ (15.89)	$2'/m'$	×	✓
0.252	$Cs_2FeCl_5.D_2O$	$C2/c$ (15)	$C2'/c$ (15.87)	$2'/m$	PT-wP	×
0.253	$Cs_2FeCl_5.D_2O$	$C2/c$ (15)	$C2$ (5.13)	2	O-wP	✓
0.254	$[C(ND_2)_3]Cu(DCOO)_3$	$Pna2_1$ (33)	$Pna2_1$ (33.144)	$mm2$	O-woP	×
0.255	$[C(ND_2)_3]Cu(DCOO)_3$	$Pna2_1$ (33)	$Pn'a'2_1$ (33.148)	$m'm'2$	BW-woP	✓
0.256	$[C(ND_2)_3]Mn(DCOO)_3$	$Pnna$ (52)	$Pn'n'a$ (52.310)	$m'm'm$	×	✓
0.257	$[C(ND_2)_3]Co(DCOO)_3$	$Pnna$ (52)	$Pn'na'$ (52.312)	$m'm'm$	×	✓
0.258	$Li_3Fe_2(PO_4)_3$	$P2_1/n$ (14)	$P2_1'/c'$ (14.79)	$2'/m'$	×	✓
0.259	$Li_3Fe_2(PO_4)_3$	$R\bar{3}$ (148)	$R\bar{3}$ (148.17)	$\bar{3}$	×	✓
0.260	$CuFePO_5$	$Pnma$ (62)	$Pnma$ (62.441)	mmm	×	×
0.261	$NiFePO_5$	$Pnma$ (62)	$Pnma$ (62.441)	mmm	×	×
0.262	$CoFePO_5$	$Pnma$ (62)	$Pnm'a'$ (62.447)	$m'm'm$	×	✓
0.263	Fe_2PO_5	$Pnma$ (62)	$Pnma$ (62.441)	mmm	×	×
0.264	$Fe_3(PO_4)_2$	$P2_1/c$ (14)	$P2_1/c'$ (14.78)	$2/m'$	PT-wP	×
0.265	$Mn_3(Co_{0.61}Mn_{0.39})N$	$Pm\bar{3}m$ (221)	$R\bar{3}$ (148.17)	$\bar{3}$	×	✓
0.266	$Na_2BaCo(VO_4)_2$	$P\bar{3}m1$ (164)	$P\bar{3}m'1$ (164.89)	$\bar{3}m'$	×	✓
0.267	$YbMnBi_2$	$P4/nmm$ (129)	$P4'/n'm'm$ (129.416)	$4'/m'm'm$	PT-wP	×
0.268	Tb_2MnNiO_6	$P2_1/c$ (14)	$P2_1'$ (4.9)	$2'$	BW-wP	✓
0.269	Tb_2MnNiO_6	$P2_1/c$ (14)	$P2_1'/c'$ (14.79)	$2'/m'$	×	✓
0.270	Tb_2MnNiO_6	$P2_1/c$ (14)	$P2_1'/c'$ (14.79)	$2'/m'$	×	✓
0.271	Tb_2MnNiO_6	$P2_1/c$ (14)	$P2_1'/c'$ (14.79)	$2'/m'$	×	✓
0.272	Tb_2MnNiO_6	$P2_1/c$ (14)	$P2_1/c$ (14.75)	$2/m$	×	✓
0.273	Mn_3ZnN	$Pm\bar{3}m$ (221)	$R\bar{3}m$ (166.97)	$\bar{3}m$	×	×
0.274	Mn_4N	$Pm\bar{3}m$ (221)	$R\bar{3}m'$ (166.101)	$\bar{3}m'$	×	✓
0.275	Mn_3AlN	$Pm\bar{3}m$ (221)	$R\bar{3}m'$ (166.101)	$\bar{3}m'$	×	✓
0.276	Mn_3AlN	$Pm\bar{3}m$ (221)	$Cmm'm'$ (65.486)	$m'm'm$	×	✓
0.277	$MgMnO_3$	$R\bar{3}$ (148)	$R\bar{3}'$ (148.19)	$\bar{3}'$	PT-wP	×
0.278	$Cu_{0.82}Mn_{1.18}As$	$P\bar{6}$ (174)	$P\bar{6}'$ (174.135)	$\bar{6}'$	BW-woP	×
0.279	Mn_3As	$P6_3/mmc$ (194)	$Cmc'm'$ (63.463)	$m'm'm$	×	✓
0.280	Mn_3As	$P6_3/mmc$ (194)	$Cm'cm'$ (63.464)	$m'm'm$	×	✓
0.281	$Co_2V_2O_7$	$P2_1/c$ (14)	$P2_1/c'$ (14.78)	$2/m'$	PT-wP	×
0.282	$U_{14}Au_51$	$P6/m$ (175)	$P6'/m$ (175.139)	$6'/m$	PT-wP	×
0.283	$U_{14}Au_51$	$P6/m$ (175)	$P6/m'$ (175.140)	$6/m'$	PT-wP	×
0.284	$KOsO_4$	$I4_1/a$ (88)	$I4_1'/a'$ (88.85)	$4'/m'$	PT-wP	×
0.285	$KRuO_4$	$I4_1/a$ (88)	$I4_1'/a'$ (88.85)	$4'/m'$	PT-wP	×
0.286	Mn_5Ge_3	$P6_3/mcm$ (193)	$P6_3/mc'm'$ (193.260)	$6/mm'm'$	×	✓
0.287	$SrCo(VO_4)(OH)$	$P2_12_12_1$ (19)	$P2_12_12_1$ (19.25)	222	O-woP	×
0.288	$NdMnO_3$	$Pnma$ (62)	$Pn'ma'$ (62.448)	$m'm'm$	×	✓
0.289	$NdMnO_3$	$Pnma$ (62)	$Pn'ma'$ (62.448)	$m'm'm$	×	✓
0.290	$CeCu_2$	$Imma$ (74)	$Im'm'a'$ (74.560)	$m'm'm'$	PT-wP	×
0.291	Tl_2NiMnO_6	$P2_1/c$ (14)	$P2_1/c$ (14.75)	$2/m$	×	✓
0.292	$NiTe_2O_5$	$Pnma$ (62)	$Pnma$ (62.441)	mmm	×	×
0.293	$(Tm_{0.7}Mn_{0.3})MnO_3$	$Pnma$ (62)	$Pnm'a'$ (62.447)	$m'm'm$	×	✓
0.294	$Cu_4(OD)_6FBr$	$Pnma$ (62)	$Pn'm'a$ (62.446)	$m'm'm$	×	✓
0.295	$Cu_2(OD)_3Cl$	$P2_1/c$ (14)	$P2_1/c$ (14.75)	$2/m$	×	✓
0.296	$Cu_2(OD)_3Cl$	$P2_1/c$ (14)	$P2_1/c$ (14.75)	$2/m$	×	✓
0.297	$NaCrGe_2O_6$	$C2/c$ (15)	$C2'/c'$ (15.89)	$2'/m'$	×	✓
0.298	$Na_2BaFe(VO_4)_2$	$C2/c$ (15)	$C2'/c'$ (15.89)	$2'/m'$	×	✓
0.299	Fe_2O_3	$Pna2_1$ (33)	$Pna'2_1'$ (33.147)	$m'm2'$	BW-woP	✓

Continued on next page

Suppl. Tab. XI – continued from previous page

BCS-ID	Formula	Parent	MSG	MPG	SHG type	LMO
0.300	Fe_2O_3	$Pna2_1$ (33)	$Pna'2_1'$ (33.147)	$m'm2'$	BW-woP	✓
0.301	Sr_2CoTeO_6	$P2_1/n$ (14)	$P2_1/c$ (14.75)	$2/m$	×	✓
0.302	$Sr_2Co_{0.9}Mg_{0.1}TeO_6$	$P2_1/n$ (14)	$P2_1/c$ (14.75)	$2/m$	×	✓
0.303	$BaCrF_5$	$P2_12_12_1$ (19)	$P2_1'2_1'2_1$ (19.27)	$2'2'2$	BW-woP	✓
0.304	$Pr_{0.5}Sr_{0.5}CoO_3$	$Imma$ (74)	$Im'm'a$ (74.558)	$m'm'm$	×	✓
0.305	$Pr_{0.5}Sr_{0.5}CoO_3$	$I4/mcm$ (140)	$Fm'm'm$ (69.524)	$m'm'm$	×	✓
0.306	$GaFeO_3$	$R3c$ (161)	Cc' (9.39)	m'	BW-woP	✓
0.307	$ScCrO_3$	$Pnma$ (62)	$Pnma$ (62.441)	mmm	×	×
0.308	$InCrO_3$	$Pnma$ (62)	$Pnma$ (62.441)	mmm	×	×
0.309	$TlCrO_3$	$Pnma$ (62)	$Pnma$ (62.441)	mmm	×	×
0.310	$NaMnFeF_6$	$P321$ (150)	$P32'1$ (150.27)	$32'$	BW-woP	✓
0.311	$CoGeO_3$	$Pbca$ (61)	$Pb'ca$ (61.435)	$m'mm$	PT-wP	×
0.312	$MnGeO_3$	$C2/c$ (15)	$C2'/c$ (15.87)	$2'/m$	PT-wP	×
0.313	$MnGeO_3$	$Pbca$ (61)	$Pb'ca$ (61.435)	$m'mm$	PT-wP	×
0.314	$ZrCo_2Ge_4O_{12}$	$P4/nbm$ (125)	$Pb'an'$ (50.282)	$m'm'm$	×	✓
0.315	$ZrMn_2Ge_4O_{12}$	$P4/nbm$ (125)	$P4'/nbm'$ (125.367)	$4'/mm'm$	×	×
0.316	$DyCrWO_6$	$Pna2_1$ (33)	$P2_1$ (4.7)	2	O-woP	✓
0.317	Ho_2CoMnO_6	$P2_1/c$ (14)	$P2_1'/c'$ (14.79)	$2'/m'$	×	✓
0.318	Tm_2CoMnO_6	$P2_1/c$ (14)	$P2_1'/c'$ (14.79)	$2'/m'$	×	✓
0.319	Tm_2CoMnO_6	$P2_1/c$ (14)	$P2_1'/c'$ (14.79)	$2'/m'$	×	✓
0.320	U_2Pd_2In	$P4/mbm$ (127)	$P4'/m'bm'$ (127.394)	$4'/m'm'm$	PT-wP	×
0.321	U_2Pd_2Sn	$P4/mbm$ (127)	$P4'/m'bm'$ (127.394)	$4'/m'm'm$	PT-wP	×
0.322	$Cu_{1.94}Mn_{1.06}BO_5$	$P2_1/c$ (14)	$P2_1'/c'$ (14.79)	$2'/m'$	×	✓
0.323	$LaCrO_3$	$Pnma$ (62)	$Pnma$ (62.441)	mmm	×	×
0.324	$CdYb_2S_4$	$Fd\bar{3}m$ (227)	$I4_1/amd$ (141.551)	$4/mmm$	×	×
0.325	$CdYb_2Se_4$	$Fd\bar{3}m$ (227)	$I4_1/amd$ (141.551)	$4/mmm$	×	×
0.326	$Nd_2Sn_2O_7$	$Fd\bar{3}m$ (227)	$Fd\bar{3}m'$ (227.131)	$m\bar{3}m'$	×	×
0.327	$CsMnF_4$	$P4/nmm$ (129)	$Pmm'n'$ (59.410)	$m'm'm$	×	✓
0.328	$KMnF_4$	$P2_1/a$ (14)	$P2_1'/c'$ (14.79)	$2'/m'$	×	✓
0.329	$RbMnF_4$	$P2_1/a$ (14)	$P\bar{1}$ (2.4)	$\bar{1}$	×	✓
0.330	$ErGe_3$	$Cmcm$ (63)	$P2_1/m'$ (11.53)	$2/m'$	PT-wP	×
0.331	$Fe_2Mo_3O_8$	$P6_3mc$ (186)	$P6_3'm'c$ (186.205)	$6'mm'$	BW-woP	×
0.332	$Co_2Mo_3O_8$	$P6_3mc$ (186)	$P6_3'm'c$ (186.205)	$6'mm'$	BW-woP	×
0.333	$Mn_2Mo_3O_8$	$P6_3mc$ (186)	$P6_3m'c'$ (186.207)	$6m'm'$	BW-woP	✓
0.334	CoF_3	$R\bar{3}c$ (167)	$R\bar{3}c$ (167.103)	$\bar{3}m$	×	×
0.335	FeF_3	$R\bar{3}c$ (167)	$C2'/c'$ (15.89)	$2'/m'$	×	✓
0.336	$NdFeO_3$	$Pnma$ (62)	$Pn'ma'$ (62.448)	$m'm'm$	×	✓
0.337	$NdFeO_3$	$Pnma$ (62)	$P2_1'/c'$ (14.79)	$2'/m'$	×	✓
0.338	$Co_2Mo_3O_8$	$P6_3mc$ (186)	$P6_3'm'c$ (186.205)	$6'mm'$	BW-woP	×
0.339	$Nd_2Hf_2O_7$	$Fd\bar{3}m$ (227)	$Fd\bar{3}m'$ (227.131)	$m\bar{3}m'$	×	×
0.340	$Nd_2Zr_2O_7$	$Fd\bar{3}m$ (227)	$Fd\bar{3}m'$ (227.131)	$m\bar{3}m'$	×	×
0.341	$DyGe_{1.75}$	$Cmmm$ (65)	$Cm'mm$ (65.483)	$m'mm$	PT-wP	×
0.342	Tb_3Ge_5	$Fdd2$ (43)	$Fdd2$ (43.224)	$mm2$	O-woP	×
0.343	$TbGe_2$	$Cmmm$ (65)	$Cm'mm$ (65.483)	$m'mm$	PT-wP	×
0.344	$ErGe_{1.83}$	$Cmc2_1$ (36)	$Cmc2_1$ (36.172)	$mm2$	O-woP	×
0.345	Tb_2C_3	$I\bar{4}3d$ (220)	$Fd'd2'$ (43.226)	$m'm2'$	BW-woP	✓
0.346	Tb_2ReC_2	$Pnma$ (62)	$Pnma'$ (62.445)	$m'mm$	PT-wP	×
0.347	Er_2ReC_2	$Pnma$ (62)	$P2_1'/c$ (14.77)	$2'/m$	PT-wP	×
0.348	Bi_2CuO_4	$P4/ncc$ (130)	$P4/n'c'c'$ (130.431)	$4/m'm'm'$	PT-wP	×
0.349	Nd_2NiO_4	$P4_2/ncm$ (138)	$P4_2/nc'm'$ (138.525)	$4/mm'm'$	×	✓
0.350	$TbAlO_3$	$Pbnm$ (62)	$Pn'm'a'$ (62.449)	$m'm'm'$	PT-wP	×

Continued on next page

Suppl. Tab. XI – continued from previous page

BCS-ID	Formula	Parent	MSG	MPG	SHG type	LMO
0.351	$TbFeO_3$	$Pbnm$ (62)	$Pn'ma'$ (62.448)	$m'm'm$	×	✓
0.352	$TbFeO_3$	$Pbnm$ (62)	$Pn'm'a$ (62.446)	$m'm'm$	×	✓
0.353	$TbFeO_3$	$Pbnm$ (62)	$P2_1'2_1'2_1$ (19.27)	$2'2'2$	BW-wP	✓
0.354	$TbCrO_3$	$Pbnm$ (62)	$Pn'm'a$ (62.446)	$m'm'm$	×	✓
0.355	$Mn_{2.85}Ga_{1.15}$	$P6_3/mmc$ (194)	$P6_3'/m'm'c$ (194.268)	$6'/m'mm'$	×	×
0.356	$Mn_{2.85}Ga_{1.15}$	$I4/mmm$ (139)	$I4/mm'm'$ (139.537)	$4/mm'm'$	×	✓
0.357	$CaFe_5O_7$	$P2_1/m$ (11)	$P2_1/m$ (11.50)	$2/m$	×	✓
0.358	$CaFe_5O_7$	$P2_1/m$ (11)	$P2_1'/m'$ (11.54)	$2'/m'$	×	✓
0.359	Mn_2ScSbO_6	$R3$ (146)	$P1$ (1.1)	1	O-woP	✓
0.360	Mn_2ScSbO_6	$P2_1/n$ (14)	$P2_1/c$ (14.75)	$2/m$	×	✓
0.361	Sr_3LiRuO_6	$R\bar{3}c$ (167)	$C2'/c'$ (15.89)	$2'/m'$	×	✓
0.362	$RbFeCl_5(D_2O)$	$Pnma$ (62)	$Pn'm'a'$ (62.449)	$m'm'm'$	PT-wP	×
0.363	$KFeCl_5(D_2O)$	$Pnma$ (62)	$Pn'm'a'$ (62.449)	$m'm'm'$	PT-wP	×
0.364	$SrCr_2As_2$	$I4/mmm$ (139)	$I4'/m'm'm$ (139.536)	$4'/m'm'm$	PT-wP	×
0.365	$BaCr_2As_2$	$I4/mmm$ (139)	$I4'/m'm'm$ (139.536)	$4'/m'm'm$	PT-wP	×
0.366	$BaCrFeAs_2$	$I4/mmm$ (139)	$I4'/m'm'm$ (139.536)	$4'/m'm'm$	PT-wP	×
0.367	$EuCr_2As_2$	$I4/mmm$ (139)	$I\bar{4}m'2'$ (119.319)	$\bar{4}2'm'$	BW-wP	✓
0.368	$(CH_3NH_3)(Co(COOH)_3$	$Pnma$ (62)	$Pn'ma'$ (62.448)	$m'm'm$	×	✓
0.369	$(CH_3NH_3)(Co(COOH)_3$	$P2_1/n$ (14)	$P2_1'/c'$ (14.79)	$2'/m'$	×	✓
0.370	$NdMnO_3$	$Pnma$ (62)	$Pn'ma'$ (62.448)	$m'm'm$	×	✓
0.371	$NdMnO_3$	$Pnma$ (62)	$Pn'ma'$ (62.448)	$m'm'm$	×	✓
0.372	$DyCrO_4$	$I4_1/a$ (88)	$C2'/c$ (15.87)	$2'/m$	PT-wP	×
0.373	$La_{0.75}Bi_{0.25}Fe_{0.5}Cr_{0.5}O_3$	$Pnma$ (62)	$Pnma$ (62.441)	mmm	×	×
0.374	YNi_4Si	$Cmmm$ (65)	$Cmm'm'$ (65.486)	$m'm'm$	×	✓
0.375	La_2CoIrO_6	$P2_1/n$ (14)	$P2_1/c$ (14.75)	$2/m$	×	✓
0.376	$LaCaFeO_4$	$Cmce$ (64)	$Cm'c'a$ (64.474)	$m'm'm$	×	✓
0.377	Mn_3Ge	$P6_3/mmc$ (194)	$Cm'cm'$ (63.464)	$m'm'm$	×	✓
0.378	UBi_2	$P4/nmm$ (129)	$P4/n'm'm'$ (129.419)	$4/m'm'm'$	PT-wP	×
0.379	$SmFeO_3$	$Pbnm$ (62)	$Pn'm'a$ (62.446)	$m'm'm$	×	✓
0.380	$SmFeO_3$	$Pnma$ (62)	$Pn'ma'$ (62.448)	$m'm'm$	×	✓
0.381	$Co_6(OH)_3(TeO_3)_4(OH)_{0.9}(H_2O)$	$P6_3mc$ (186)	$P6_3'mc'$ (186.206)	$6'mm'$	BW-woP	×
0.382	$LiMnPO_4$	$Pnma$ (62)	$Pn'm'a'$ (62.449)	$m'm'm'$	PT-wP	×
0.383	$LiCoPO_4$	$Pnma$ (62)	$Pnma'$ (62.445)	$m'mm$	PT-wP	×
0.384	$LiCoPO_4$	$Pnma$ (62)	$P2_1'/c$ (14.77)	$2'/m$	PT-wP	×
0.385	$LiCoPO_4$	$Pnma$ (62)	$P2_1/c'$ (14.78)	$2/m'$	PT-wP	×
0.386	Fe_3BO_5	$Pnma$ (62)	$Pnm'a$ (62.444)	$m'mm$	PT-wP	×
0.387	Fe_3BO_5	$Pnma$ (62)	$Pm'c2_1'$ (26.68)	$m'm2'$	BW-wP	✓
0.388	$Co_3Al_2Si_3O_{12}$	$Ia\bar{3}d$ (230)	$I4_1/a'cd$ (142.563)	$4/m'mm$	PT-wP	×
0.389	$Fe_{1.5}Mn_{1.5}BO_5$	$Pbam$ (55)	$Pbam$ (55.353)	mmm	×	×
0.390	$Y_2SrCu_{0.6}Co_{1.4}O_{6.5}$	$Ibam$ (72)	$Ib'a'm$ (72.543)	$m'm'm$	×	✓
0.391	$Y_2SrCu_{0.6}Co_{1.4}O_{6.5}$	$Ibam$ (72)	$Ib'a'm$ (72.543)	$m'm'm$	×	✓
0.392	$Fe_3(PO_4)_2(OH)_2$	$P2_1/c$ (14)	$P2_1/c$ (14.75)	$2/m$	×	✓
0.393	$Cu_4(OH)_6FBr$	$P6_3/m$ (176)	$P2_1'/m'$ (11.54)	$2'/m'$	×	✓
0.394	$Cu_2CdB_2O_6$	$P2_1/c$ (14)	$P2_1/c'$ (14.78)	$2/m'$	PT-wP	×
0.395	$MnPtGa$	$P6_3/mmc$ (194)	$Cm'c'm$ (63.462)	$m'm'm$	×	✓
0.396	$MnPtGa$	$P6_3/mmc$ (194)	$Cm'c'm$ (63.462)	$m'm'm$	×	✓
0.397	$Mn_3Si_2Te_6$	$P\bar{3}1c$ (163)	$C2'/c'$ (15.89)	$2'/m'$	×	✓
0.398	Ca_2RuO_4	$Pbca$ (61)	$Pbca$ (61.433)	mmm	×	×
0.399	$FeOOH$	$Pbnm$ (62)	$Pnma'$ (62.445)	$m'mm$	PT-wP	×
0.400	$Sr_2Fe_{1.9}Co_{0.1}O_{5.5}$	$Cmmm$ (65)	$Cm'm'm'$ (65.487)	$m'm'm'$	PT-wP	×
0.401	$Sr_4Fe_4O_{11}$	$Cmmm$ (65)	$Cm'm'm'$ (65.487)	$m'm'm'$	PT-wP	×

Continued on next page

Suppl. Tab. XI – continued from previous page

BCS-ID	Formula	Parent	MSG	MPG	SHG type	LMO
0.402	$Sr_4Fe_4O_{11}$	$Cmmm$ (65)	$Cmm'm'$ (65.486)	$m'm'm$	×	✓
0.403	$NdCo_2$	$Fd\bar{3}m$ (227)	$Imm'a'$ (74.559)	$m'm'm$	×	✓
0.404	Sr_3NaRuO_6	$R\bar{3}c$ (167)	$C2'/c'$ (15.89)	$2'/m'$	×	✓
0.405	$CsCoF_4$	$I\bar{4}c2$ (120)	$I\bar{4}'$ (82.41)	$\bar{4}'$	BW-woP	×
0.406	$GdNiSi_3$	$Cmmm$ (65)	$Cmmm'$ (65.484)	$m'mm$	PT-wP	×
0.407	$NdSi$	$Pnma$ (62)	$Pn'm'a$ (62.446)	$m'm'm$	×	✓
0.408	$PrSi$	$Pnma$ (62)	$Pnm'a'$ (62.447)	$m'm'm$	×	✓
0.409	$TmNi$	$Pnma$ (62)	$Pn'm'a$ (62.446)	$m'm'm$	×	✓
0.410	$GdAlO_3$	$Pbnm$ (62)	$Pn'm'a'$ (62.449)	$m'm'm'$	PT-wP	×
0.411	Tb_5Ge_4	$Pnma$ (62)	$Pnm'a$ (62.444)	$m'mm$	PT-wP	×
0.412	Tb_5Ge_4	$Pnma$ (62)	$Pnm'a$ (62.444)	$m'mm$	PT-wP	×
0.413	$UGeSe$	$I4/mmm$ (139)	$I4/m'm'm'$ (139.539)	$4/m'm'm'$	PT-wP	×
0.414	$AlFe_2B_2$	$Cmmm$ (65)	$Cmm'm'$ (65.486)	$m'm'm$	×	✓
0.415	$EuFe_2P_2$	$I4/mmm$ (139)	$C2'/m'$ (12.62)	$2'/m'$	×	✓
0.416	$LaCrO_3$	$R\bar{3}c$ (167)	$R\bar{3}c$ (167.103)	$\bar{3}m$	×	×
0.417	$LaCrO_3$	$Pnma$ (62)	$Pn'ma'$ (62.448)	$m'm'm$	×	✓
0.418	$K_{0.8}Fe_{1.8}Se_2$	$I4/m$ (87)	$I4/m'$ (87.78)	$4/m'$	PT-wP	×
0.419	$ErGe_2O_7$	$P4_12_12$ (92)	$P4_1'2_12'$ (92.113)	$4'22'$	BW-woP	×
0.420	Sr_2LuRuO_6	$P2_1/n$ (14)	$P2_1/c$ (14.75)	$2/m$	×	✓
0.421	$EuMnSb_2$	$Pnma$ (62)	$Pn'm'a'$ (62.449)	$m'm'm'$	PT-wP	×
0.422	$EuMnSb_2$	$Pnma$ (62)	$P2_1/m'$ (11.53)	$2/m'$	PT-wP	×
0.423	$EuMnSb_2$	$Pnma$ (62)	$Pn'm'a'$ (62.449)	$m'm'm'$	PT-wP	×
0.424	$EuMnSb_2$	$Pnma$ (62)	$Pn'm'a'$ (62.449)	$m'm'm'$	PT-wP	×
0.425	$Na_2CoP_2O_7$	$Pna2_1$ (33)	$Pn'a2_1'$ (33.146)	$m'm2'$	BW-woP	✓
0.426	$EuMnBi_2$	$I4/mmm$ (139)	$I4'/m'm'm$ (139.536)	$4'/m'm'm$	PT-wP	×
0.427	$Sm_2Ti_2O_7$	$Fd\bar{3}m$ (227)	$Fd\bar{3}m'$ (227.131)	$m\bar{3}m'$	×	×
0.428	$BaMn_2Si_2O_7$	$C2/c$ (15)	$C2/c$ (15.85)	$2/m$	×	✓
0.429	$CaCr_{0.86}Fe_{3.14}As_3$	$Pnma$ (62)	$Pn'ma$ (62.443)	$m'mm$	PT-wP	×
0.430	Yb_3Pt_4	$R\bar{3}$ (148)	$R\bar{3}'$ (148.19)	$\bar{3}'$	PT-wP	×
0.431	CuB_2O_4	$I\bar{4}2d$ (122)	$P1$ (1.1)	1	O-woP	✓
0.432	$KMnF_3$	$Pnma$ (62)	$Pn'ma'$ (62.448)	$m'm'm$	×	✓
0.433	$KMnF_3$	$I4/mcm$ (140)	$I4/mcm$ (140.541)	$4/mmm$	×	×
0.434	K_2ReI_6	$P2_1/n$ (14)	$P2_1/c$ (14.75)	$2/m$	×	✓
0.435	$Pb_5Fe_3TiO_{11}Cl$	$P4/mmm$ (123)	P_Bmma (51.302)	$mmm1'$	×	×
0.436	$TbNi_4Si$	$Cmmm$ (65)	$Cmm'm'$ (65.486)	$m'm'm$	×	✓
0.437	Ho_3NiGe_2	$Pnma$ (62)	$Pnm'a'$ (62.447)	$m'm'm$	×	✓
0.438	Pr_3CoGe_2	$Pnma$ (62)	$Pnm'a'$ (62.447)	$m'm'm$	×	✓
0.439	Tb_3NiGe_2	$Pnma$ (62)	$Pn'ma'$ (62.448)	$m'm'm$	×	✓
0.440	$SrCuTe_2O_6$	$P4_132$ (213)	$P4_132$ (213.63)	432	×	×
0.441	$Fe_4Nb_2O_9$	$P\bar{3}c1$ (165)	$C2/c'$ (15.88)	$2/m'$	PT-wP	×
0.442	$Fe_4Nb_2O_9$	$C2/c$ (15)	$C2/c'$ (15.88)	$2/m'$	PT-wP	×
0.443	$Fe_4Nb_2O_9$	$P\bar{3}c1$ (165)	$C2/c'$ (15.88)	$2/m'$	PT-wP	×
0.444	$YbCl_3$	$C2/m$ (12)	$C2'/m$ (12.60)	$2'/m$	PT-wP	×
0.445	$MnCoGe$	$Pnma$ (62)	$Pn'm'a$ (62.446)	$m'm'm$	×	✓
0.446	$MnCoGeB_{0.05}$	$P6_3/mmc$ (194)	$Cm'c'm$ (63.462)	$m'm'm$	×	✓
0.447	$MnCoGeB_{0.05}$	$P6_3/mmc$ (194)	$P6_3/mm'c'$ (194.270)	$6/mm'm'$	×	✓
0.448	Ce_4Ge_3	$I\bar{4}3d$ (220)	$I\bar{4}2d$ (122.333)	$\bar{4}2m$	O-woP	×
0.449	Tb_2Pt	$Pnma$ (62)	$P2_1'/m'$ (11.54)	$2'/m'$	×	✓
0.450	Nd_5Ge_4	$Pnma$ (62)	$Pnm'a'$ (62.447)	$m'm'm$	×	✓
0.451	$DyRuAsO$	$Pmmn$ (59)	$Pm'mn$ (59.407)	$m'mm$	PT-wP	×
0.452	$TbRuAsO$	$P4/nmm$ (129)	$Pm'mn$ (59.407)	$m'mm$	PT-wP	×

Continued on next page

Suppl. Tab. XI – continued from previous page

BCS-ID	Formula	**Parent**	**MSG**	**MPG**	**SHG type**	**LMO**
0.453	$DyCoSi_2$	$Cmcm$ (63)	$Cm'cm$ (63.459)	$m'mm$	PT-wP	×
0.454	PrScSb	$I4/mmm$ (139)	P_I4/mnc (128.410)	$4/mmm1'$	×	×
0.455	$RbFeO_2$	$Pbca$ (61)	$Pb'c'a'$ (61.437)	$m'm'm'$	PT-wP	×
0.456	$RbFeO_2$	$Fd\bar{3}m$ (227)	$I4_1'/a'm'd$ (141.556)	$4'/m'm'm$	PT-wP	×
0.457	$CsFeO_2$	$Pbca$ (61)	$Pb'c'a'$ (61.437)	$m'm'm'$	PT-wP	×
0.458	$CsFeO_2$	$Fd\bar{3}m$ (227)	$I4_1'/a'm'd$ (141.556)	$4'/m'm'm$	PT-wP	×
0.459	$KFeO_2$	$Pbca$ (61)	$Pb'ca$ (61.435)	$m'mm$	PT-wP	×
0.460	$KFeO_2$	$Pbca$ (61)	$Pb'ca$ (61.435)	$m'mm$	PT-wP	×
0.461	$CoRh_2O_4$	$Fd\bar{3}m$ (227)	$I4_1'/a'm'd$ (141.556)	$4'/m'm'm$	PT-wP	×
0.462	$MnAl_2O_4$	$Fd\bar{3}m$ (227)	$I4_1'/a'm'd$ (141.556)	$4'/m'm'm$	PT-wP	×
0.463	Co_3O_4	$Fd\bar{3}m$ (227)	$I4_1'/a'm'd$ (141.556)	$4'/m'm'm$	PT-wP	×
0.464	$BaMn_2P_2$	$I4/mmm$ (139)	$I4'/m'm'm$ (139.536)	$4'/m'm'm$	PT-wP	×
0.465	$HoCr_2Si_2$	$I4/mmm$ (139)	$I4'/m'm'm$ (139.536)	$4'/m'm'm$	PT-wP	×
0.466	$ThCr_2Si_2$	$I4/mmm$ (139)	$Im'mm$ (71.535)	$m'mm$	PT-wP	×
0.467	$TbPO_4$	$I4_1/amd$ (141)	$I4_1'/a'm'd$ (141.556)	$4'/m'm'm$	PT-wP	×
0.468	ErB_4	$P4/mbm$ (127)	$Pb'am$ (55.355)	$m'mm$	PT-wP	×
0.469	TbB_4	$P4/mbm$ (127)	$Pb'a'm'$ (55.359)	$m'm'm'$	PT-wP	×
0.470	$BaMn_2Sb_2$	$I4/mmm$ (139)	$I4'/m'm'm$ (139.536)	$4'/m'm'm$	PT-wP	×
0.471	$Ba_2Mn_3Sb_2O_2$	$I4/mmm$ (139)	$I4'/m'm'm$ (139.536)	$4'/m'm'm$	PT-wP	×
0.472	$LaMn_2Si_2$	$I4/mmm$ (139)	$I4'/m'm'm$ (139.536)	$4'/m'm'm$	PT-wP	×
0.473	$LaMn_2Si_2$	$I4/mmm$ (139)	$Im'm2'$ (44.231)	$m'm2'$	BW-wP	✓
0.474	$EuMn_2Ge_2$	$I4/mmm$ (139)	$I4'/m'm'm$ (139.536)	$4'/m'm'm$	PT-wP	×
0.475	Sr_2TbIrO_6	$P2_1/n$ (14)	$P2_1/c$ (14.75)	$2/m$	×	✓
0.476	$Cs_2[FeCl_5(H_2O)]$	$I2/c$ (15)	$C2'/c$ (15.87)	$2'/m$	PT-wP	×
0.477	$Mn_4Ta_2O_9$	$P\bar{3}c1$ (165)	$P\bar{3}'c'1$ (165.94)	$\bar{3}'m'$	PT-wP	×
0.478	$SmCrO_3$	$Pnma$ (62)	$Pnma$ (62.441)	mmm	×	×
0.479	$SmCrO_3$	$Pnma$ (62)	$Pn'ma'$ (62.448)	$m'm'm$	×	✓
0.480	HoNi	$Pnma$ (62)	$Pnm'a'$ (62.447)	$m'm'm$	×	✓
0.481	HoNi	$Pnma$ (62)	$P2_1'/c'$ (14.79)	$2'/m'$	×	✓
0.482	$SrMn_2As_2$	$P\bar{3}m1$ (164)	$C2'/m$ (12.60)	$2'/m$	PT-wP	×
0.483	$YbMn_2Sb_2$	$P\bar{3}m1$ (164)	$P\bar{1}'$ (2.6)	$\bar{1}'$	PT-wP	×
0.484	U_2N_2S	$P\bar{3}m1$ (164)	$P\bar{3}'m'1$ (164.88)	$\bar{3}'m'$	PT-wP	×
0.485	U_2N_2Se	$P\bar{3}m1$ (164)	$P\bar{3}'m'1$ (164.88)	$\bar{3}'m'$	PT-wP	×
0.486	$ErCr_2Si_2$	$I4/mmm$ (139)	$I4'/m'm'm$ (139.536)	$4'/m'm'm$	PT-wP	×
0.487	$ErCr_2Si_2$	$I4/mmm$ (139)	$Im'm'2$ (44.232)	$m'm'2$	BW-wP	✓
0.488	$YbMnO_3$	$P6_3cm$ (185)	$P6_3'c'm$ (185.199)	$6'mm'$	BW-woP	×
0.489	$YbMnO_3$	$P6_3cm$ (185)	$P6_3'c'm$ (185.199)	$6'mm'$	BW-woP	×
0.490	$YbMnO_3$	$P6_3cm$ (185)	$P6_3c'm'$ (185.201)	$6m'm'$	BW-woP	✓
0.491	NdB_4	$P4/mbm$ (127)	$P4/m'$ (83.46)	$4/m'$	PT-wP	×
0.492	NdB_4	$P4/mbm$ (127)	$P2_1'/c$ (14.77)	$2'/m$	PT-wP	×
0.493	$Ho(Co_{0.667}Ga_{0.333})_2$	$P6_3/mmc$ (194)	$C2'/c'$ (15.89)	$2'/m'$	×	✓
0.494	$Er(Co_{0.667}Ga_{0.333})_2$	$P6_3/mmc$ (194)	$P6_3/mm'c'$ (194.270)	$6/mm'm'$	×	✓
0.495	$LaMn_2Si_2$	$I4/mmm$ (139)	$Im'm2'$ (44.231)	$m'm2'$	BW-wP	✓
0.496	$LaMn_2Si_2$	$I4/mmm$ (139)	$Im'm2'$ (44.231)	$m'm2'$	BW-wP	✓
0.497	$LaMn_2Si_2$	$I4/mmm$ (139)	$Im'm2'$ (44.231)	$m'm2'$	BW-wP	✓
0.498	$LaMn_2Si_2$	$I4/mmm$ (139)	$I4'/m'm'm$ (139.536)	$4'/m'm'm$	PT-wP	×
0.499	UCr_2Si_2C	$P4/mmm$ (123)	$Pm'm'm$ (47.252)	$m'm'm$	×	✓
0.500	$Ca_2FeMn_{0.5}W_{0.5}O_6$	$P2_1/n$ (14)	$P2_1'/c'$ (14.79)	$2'/m'$	×	✓
0.501	$LiFe_2F_6$	$P4_2/mnm$ (136)	$P4_2'/mnm'$ (136.499)	$4'/mm'm$	×	×
0.502	$La_2Ni_{1.19}Os_{0.81}O_6$	$P2_1/c$ (14)	$P2_1'/c'$ (14.79)	$2'/m'$	×	✓
0.503	$K_{1.62}Fe_4O_{6.62}(OH)_{0.38}$	$P\bar{3}1c$ (163)	$P\bar{3}1c$ (163.79)	$\bar{3}m$	×	×

Continued on next page

Suppl. Tab. XI – continued from previous page

BCS-ID	Formula	Parent	MSG	MPG	SHG type	LMO
0.504	$NaCrSi_2O_6$	$C2/c$ (15)	$P\bar{1}'$ (2.6)	$\bar{1}'$	PT-wP	×
0.505	$Pb_2VO(PO_4)_2$	$P2_1/a$ (14)	$P2_1/c'$ (14.78)	$2/m'$	PT-wP	×
0.506	$Cs_2Cu_3SnF_{12}$	$P2_1/n$ (14)	$P2_1'/c'$ (14.79)	$2'/m'$	×	✓
0.507	$Mn_4Nb_2O_9$	$P\bar{3}c1$ (165)	$P\bar{3}'c'1$ (165.94)	$\bar{3}'m'$	PT-wP	×
0.508	$FeMnO_3$	$Ia\bar{3}$ (206)	$Ib'c'a$ (73.551)	$m'm'm$	×	✓
0.509	$BaFe_{12}O_{19}$	$P6_3/mmc$ (194)	$P6_3/mm'c'$ (194.270)	$6/mm'm'$	×	✓
0.510	Mn_2NiReO_6	$P2_1/n$ (14)	$P2_1/c$ (14.75)	$2/m$	×	✓
0.511	$Co_4Ta_2O_9$	$P\bar{3}c1$ (165)	$C2'/c$ (15.87)	$2'/m$	PT-wP	×
0.512	Mn_3As_2	$C2/m$ (12)	$C2/m$ (12.58)	$2/m$	×	✓
0.513	$YRuO_3$	$Pnma$ (62)	$Pn'ma'$ (62.448)	$m'm'm$	×	✓
0.514	$CoFe_3O_5$	$Cmcm$ (63)	$Cm'cm'$ (63.464)	$m'm'm$	×	✓
0.515	$CoFe_3O_5$	$Cmcm$ (63)	$P2_1'/m'$ (11.54)	$2'/m'$	×	✓
0.516	$BaMg_2Fe_{16}O_{27}$	$P6_3/mmc$ (194)	$P6_3/mm'c'$ (194.270)	$6/mm'm'$	×	✓
0.517	$BaCo_2Fe_{16}O_{27}$	$P6_3/mmc$ (194)	$P6_3/mm'c'$ (194.270)	$6/mm'm'$	×	✓
0.518	$TbCr_2Si_2$	$I4/mmm$ (139)	$I4'/m'm'm$ (139.536)	$4'/m'm'm$	PT-wP	×
0.519	$HoCr_2Si_2$	$I4/mmm$ (139)	$I4'/m'm'm$ (139.536)	$4'/m'm'm$	PT-wP	×
0.520	$TbCoO_3$	$Pbnm$ (62)	$Pnm'a$ (62.444)	$m'mm$	PT-wP	×
0.521	$DyCoO_3$	$Pbnm$ (62)	$Pn'm'a'$ (62.449)	$m'm'm'$	PT-wP	×
0.522	$La_2O_3FeMnSe_2$	$I4/mmm$ (139)	$Im'm'm$ (71.536)	$m'm'm$	×	✓
0.523	$CaMn_2Sb_2$	$P\bar{3}m1$ (164)	$P\bar{1}'$ (2.6)	$\bar{1}'$	PT-wP	×
0.524	$MnPSe_3$	$R\bar{3}$ (148)	$P\bar{1}'$ (2.6)	$\bar{1}'$	PT-wP	×
0.525	$NaCeO_2$	$I4_1/amd$ (141)	$I4_1'/a'm'd$ (141.556)	$4'/m'm'm$	PT-wP	×
0.526	$Mn_4Ta_2O_9$	$P\bar{3}c1$ (165)	$P\bar{3}'c'1$ (165.94)	$\bar{3}'m'$	PT-wP	×
0.527	$Er_2Si_2O_7$	$C2/m$ (12)	$C2'/m$ (12.60)	$2'/m$	PT-wP	×
0.528	$CrSb$	$P6_3/mmc$ (194)	$P6_3'/m'm'c$ (194.268)	$6'/m'mm'$	×	×
0.529	$Co_4Nb_2O_9$	$P\bar{3}c1$ (165)	$C2/c'$ (15.88)	$2/m'$	PT-wP	×
0.530	$SrCuTe_2O_6$	$P4_132$ (213)	$P4_132$ (213.63)	432	×	×
0.531	$Sr_{0.7}Tb_{0.3}CoO_{2.9}$	$I4/mmm$ (139)	$I4'/mmm'$ (139.535)	$4'/mm'm$	×	×
0.532	$Sr_{0.7}Ho_{0.3}CoO_{2.7}$	$I4/mmm$ (139)	$I4'/mmm'$ (139.535)	$4'/mm'm$	×	×
0.533	$Sr_{0.7}Er_{0.3}CoO_{2.8}$	$I4/mmm$ (139)	$I4'/mmm'$ (139.535)	$4'/mm'm$	×	×
0.534	$Tb_{0.55}Sr_{0.45}MnO_3$	$Pnma$ (62)	$Pnm'a'$ (62.447)	$m'm'm$	×	✓
0.535	$Tb_{0.55}Sr_{0.45}MnO_3$	$Pnma$ (62)	$Pnm'a'$ (62.447)	$m'm'm$	×	✓
0.536	$Tb_{0.55}Sr_{0.45}MnO_3$	$Pnma$ (62)	$Pnm'a'$ (62.447)	$m'm'm$	×	✓
0.537	$CaMn_{0.7}Co_{1.3}ReO_6$	$P4_2/n$ (86)	$P42/n$ (86.67)	$4/m$	×	✓
0.538	$CaMn_{1.2}Ni_{0.8}ReO_6$	$P4_2/n$ (86)	$P42/n$ (86.67)	$4/m$	×	✓
0.539	$Mn_2Fe_{0.8}Mo_{1.2}O_6$	$P2_1/n$ (14)	$P2_1/c$ (14.75)	$2/m$	×	✓
0.540	$Mn_2Fe_{0.8}Mo_{1.2}O_6$	$P2_1/n$ (14)	$P2_1/c$ (14.75)	$2/m$	×	✓
0.541	Mn_2FeReO_6	$P2_1/c$ (14)	$P2_1'/c'$ (14.79)	$2'/m'$	×	✓
0.542	Mn_2FeReO_6	$P2_1/c$ (14)	$P\bar{1}$ (2.4)	$\bar{1}$	×	✓
0.543	Mn_2FeReO_6	$P2_1/c$ (14)	$P\bar{1}$ (2.4)	$\bar{1}$	×	✓
0.544	Mn_2FeReO_6	$P2_1/c$ (14)	$P\bar{1}$ (2.4)	$\bar{1}$	×	✓
0.545	Mn_2FeReO_6	$P2_1/c$ (14)	$P\bar{1}$ (2.4)	$\bar{1}$	×	✓
0.546	Mn_2FeReO_6	$P2_1/c$ (14)	$P2_1'/c'$ (14.79)	$2'/m'$	×	✓
0.547	Mn_2FeReO_6	$P2_1/c$ (14)	$P2_1'/c'$ (14.79)	$2'/m'$	×	✓
0.548	Mn_2FeReO_6	$P2_1/c$ (14)	$P\bar{1}$ (2.4)	$\bar{1}$	×	✓
0.549	Mn_2FeReO_6	$P2_1/c$ (14)	$P\bar{1}$ (2.4)	$\bar{1}$	×	✓
0.550	Mn_3ReO_6	$P2_1/c$ (14)	$P_S\bar{1}$ (2.7)	$\bar{1}1'$	×	×
0.551	Mn_3ReO_6	$P2_1/c$ (14)	$P_S\bar{1}$ (2.7)	$\bar{1}1'$	×	×
0.552	Pb_2MnO_4	$P\bar{4}2_1c$ (114)	$P\bar{4}'2_1c'$ (114.278)	$\bar{4}'2m'$	BW-woP	×
0.553	K_2ReI_6	$P2_1/n$ (14)	$P2_1/c$ (14.75)	$2/m$	×	✓
0.554	Co_2MnSi	$Fm\bar{3}m$ (225)	$I4/mm'm'$ (139.537)	$4/mm'm'$	×	✓

Continued on next page

Suppl. Tab. XI – continued from previous page

BCS-ID	Formula	Parent	MSG	MPG	SHG type	LMO
0.555	$Ho_{0.05}Bi_{0.95}FeO_3$	$R3c$ (161)	$R3c$ (161.69)	$3m$	O-woP	×
0.556	$Ho_{0.1}Bi_{0.9}FeO_3$	$R3c$ (161)	$R3c$ (161.69)	$3m$	O-woP	×
0.557	$Ho_{0.15}Bi_{0.85}FeO_3$	$R3c$ (161)	Cc (9.37)	m	O-woP	✓
0.558	$Ho_{0.2}Bi_{0.8}FeO_3$	$R3c$ (161)	Cc (9.37)	m	O-woP	✓
0.559	$Ho_{0.15}Bi_{0.85}FeO_3$	$Pnma$ (62)	$Pn'ma'$ (62.448)	$m'm'm$	×	✓
0.560	$Ho_{0.2}Bi_{0.8}FeO_3$	$Pnma$ (62)	$Pn'ma'$ (62.448)	$m'm'm$	×	✓
0.561	$NdNiGe_2$	$Cmcm$ (63)	$Cm'c'm$ (63.462)	$m'm'm$	×	✓
0.562	$Ce_2Ni_3Ge_5$	$Ibam$ (72)	P_Ibcn (60.432)	$mmm1'$	×	×
0.563	$Ce_2Ni_3Ge_5$	$Ibam$ (72)	P_Iccn (56.376)	$mmm1'$	×	×
0.564	$U_2Rh_3Si_5$	$I2/c$ (15)	P_C2/c (13.74)	$2/m1'$	×	×
0.565	$Ce_2Ni_3Ge_5$	$Ibam$ (72)	P_Ibcn (60.432)	$mmm1'$	×	×
0.566	$TbNiGe_2$	$Cmcm$ (63)	$Cm'cm$ (63.459)	$m'mm$	PT-wP	×
0.567	$HoNi_{0.64}Ge_2$	$Cmcm$ (63)	$Cm'cm$ (63.459)	$m'mm$	PT-wP	×
0.568	$TbNi_{0.4}Ge_2$	$Cmcm$ (63)	$Cm'cm$ (63.459)	$m'mm$	PT-wP	×
0.569	$TbCu_{0.4}Ge_2$	$Cmcm$ (63)	$Cm'cm$ (63.459)	$m'mm$	PT-wP	×
0.570	$Li_{0.5}FeCr_{1.5}O_4$	$Fd\bar{3}m$ (227)	$I4_1/am'd'$ (141.557)	$4/mm'm'$	×	✓
0.571	$CoSO_4$	$Pbnm$ (62)	$Pnma$ (62.441)	mmm	×	×
0.572	Na_2NiCrF_7	$Imma$ (74)	$Im'm'a$ (74.558)	$m'm'm$	×	✓
0.573	Na_2NiCrF_7	$Imma$ (74)	$Im'm'a$ (74.558)	$m'm'm$	×	✓
0.574	$MnFeF_5(H_2O)_2$	$Imm2$ (44)	$C2'$ (5.15)	$2'$	BW-woP	✓
0.575	$ZnFeF_5(H_2O)_2$	$Imm2$ (44)	$Imm2$ (44.229)	$mm2$	O-woP	×
0.576	Cr_2F_5	$C2/c$ (15)	$C2/c$ (15.85)	$2/m$	×	✓
0.577	$BaMnFeF_7$	$P2_1/c$ (14)	$P2_1'/c'$ (14.79)	$2'/m'$	×	✓
0.578	$NaBaFe_2F_9$	$P2_1/c$ (14)	$P2_1/c$ (14.75)	$2/m$	×	✓
0.579	Na_2NiFeF_7	$Imma$ (74)	$Imm'a'$ (74.559)	$m'm'm$	×	✓
0.580	Na_2NiFeF_7	$Imma$ (74)	$Imm'a'$ (74.559)	$m'm'm$	×	✓
0.581	FeF_3	$R\bar{3}c$ (167)	$C2'/c'$ (15.89)	$2'/m'$	×	✓
0.582	$Fe_3F_8(H_2O)_2$	$C2/m$ (12)	$C2'/m'$ (12.62)	$2'/m'$	×	✓
0.583	$Fe_2F_5(H_2O)_2$	$Imma$ (74)	$Imm'a'$ (74.559)	$m'm'm$	×	✓
0.584	$Fe_2F_5(H_2O)_2$	$Imma$ (74)	$C2'/c'$ (15.89)	$2'/m'$	×	✓
0.585	$YbCl_3$	$C2/m$ (12)	$C2'/m$ (12.60)	$2'/m$	PT-wP	×
0.586	$YCrO_3$	$Pbnm$ (62)	$Pn'ma'$ (62.448)	$m'm'm$	×	✓
0.587	$TmCrO_3$	$Pbnm$ (62)	$Pn'ma'$ (62.448)	$m'm'm$	×	✓
0.588	$PrCrO_3$	$Pbnm$ (62)	$Pn'ma'$ (62.448)	$m'm'm$	×	✓
0.589	$NdCrO_3$	$Pbnm$ (62)	$P2_1/m$ (11.50)	$2/m$	×	✓
0.590	$ErCrO_3$	$Pbnm$ (62)	$P2_1/m$ (11.50)	$2/m$	×	✓
0.591	$ErCrO_3$	$Pbnm$ (62)	$Pn'ma'$ (62.448)	$m'm'm$	×	✓
0.592	$DyCrO_3$	$Pbnm$ (62)	$Pn'm'a$ (62.446)	$m'm'm$	×	✓
0.593	UPSe	$P4/nmm$ (129)	$P4/nm'm'$ (129.417)	$4/mm'm'$	×	✓
0.594	UAsS	$P4/nmm$ (129)	$P4/nm'm'$ (129.417)	$4/mm'm'$	×	✓
0.595	UPTe	$I4/mmm$ (139)	$I4/mm'm'$ (139.537)	$4/mm'm'$	×	✓
0.596	UAsTe	$I4/mmm$ (139)	$I4/mm'm'$ (139.537)	$4/mm'm'$	×	✓
0.597	$MnBi_8Te_{13}$	$R\bar{3}m$ (166)	$R\bar{3}m'$ (166.101)	$\bar{3}m'$	×	✓
0.598	$AlCr_2$	$I4/mmm$ (139)	P_A2_1/c (14.83)	$2/m1'$	×	×
0.599	CaMnSi	$P4/nmm$ (129)	$P4'/n'm'm$ (129.416)	$4'/m'm'm$	PT-wP	×
0.600	CaMnSi	$P4/nmm$ (129)	$P4'/n'm'm$ (129.416)	$4'/m'm'm$	PT-wP	×
0.601	CaMnGe	$P4/nmm$ (129)	$P2_1/m'$ (11.53)	$2/m'$	PT-wP	×
0.602	CaMnGe	$P4/nmm$ (129)	$P2_1/m'$ (11.53)	$2/m'$	PT-wP	×
0.603	$CaMn_2Ge_2$	$I4/mmm$ (139)	$I4'/m'm'm$ (139.536)	$4'/m'm'm$	PT-wP	×
0.604	$CaMn_2Ge_2$	$I4/mmm$ (139)	$I4'/m'm'm$ (139.536)	$4'/m'm'm$	PT-wP	×
0.605	$BaMn_2Ge_2$	$I4/mmm$ (139)	$I4'/m'm'm$ (139.536)	$4'/m'm'm$	PT-wP	×

Continued on next page

Suppl. Tab. XI – continued from previous page

BCS-ID	Formula	Parent	MSG	MPG	SHG type	LMO
0.606	$BaMn_2Ge_2$	$I4/mmm$ (139)	$I4'/m'm'm$ (139.536)	$4'/m'm'm$	PT-wP	×
0.607	RuO_2	$P4_2/mnm$ (136)	$P4_2'/mnm'$ (136.499)	$4'/mm'm$	×	×
0.608	$PrMnO_3$	$Pbnm$ (62)	$Pn'ma'$ (62.448)	$m'm'm$	×	✓
0.609	$NdMnO_3$	$Pbnm$ (62)	$P2_1/m$ (11.50)	$2/m$	×	✓
0.610	$Pr_{0.95}K_{0.05}MnO_3$	$Pbnm$ (62)	$Pn'ma'$ (62.448)	$m'm'm$	×	✓
0.611	$BaMnSb_2$	$I4/mmm$ (139)	$I4'/m'm'm$ (139.536)	$4'/m'm'm$	PT-wP	×
0.612	Cu_2OSO_4	$C2/m$ (12)	$C2/m$ (12.58)	$2/m$	×	✓
0.613	$FeCr_2S_4$	$Fd\bar{3}m$ (227)	$I4_1/am'd'$ (141.557)	$4/mm'm'$	×	✓
0.614	$FeCr_2S_4$	$Fd\bar{3}m$ (227)	$I4_1/am'd'$ (141.557)	$4/mm'm'$	×	✓
0.615	$FeCr_2S_4$	$Fd\bar{3}m$ (227)	$I4_1/am'd'$ (141.557)	$4/mm'm'$	×	✓
0.616	HoB_2	$P6/mmm$ (191)	$C2'/m'$ (12.62)	$2'/m'$	×	✓
0.617	KMnSb	$P4/nmm$ (129)	$P4'/n'm'm$ (129.416)	$4'/m'm'm$	PT-wP	×
0.618	KMnBi	$P4/nmm$ (129)	$P4'/n'm'm$ (129.416)	$4'/m'm'm$	PT-wP	×
0.619	LaMnAsO	$P4/nmm$ (129)	$P4'/n'm'm$ (129.416)	$4'/m'm'm$	PT-wP	×
0.620	NdMnAsO	$P4/nmm$ (129)	$P4'/n'm'm$ (129.416)	$4'/m'm'm$	PT-wP	×
0.621	NdMnAsO	$P4/nmm$ (129)	$Pm'mn$ (59.407)	$m'mm$	PT-wP	×
0.622	NdMnAsO	$P4/nmm$ (129)	$Pm'mn$ (59.407)	$m'mm$	PT-wP	×
0.623	NdMnAsO	$P4/nmm$ (129)	$P4'/n'm'm$ (129.416)	$4'/m'm'm$	PT-wP	×
0.624	LaMnAsO	$P4/nmm$ (129)	$P4'/n'm'm$ (129.416)	$4'/m'm'm$	PT-wP	×
0.625	U_2Pd_2In	$P4/mbm$ (127)	$P4'/m'bm'$ (127.394)	$4'/m'm'm$	PT-wP	×
0.626	NaMnP	$P4/nmm$ (129)	$P4'/n'm'm$ (129.416)	$4'/m'm'm$	PT-wP	×
0.627	NaMnP	$P4/nmm$ (129)	$P4'/n'm'm$ (129.416)	$4'/m'm'm$	PT-wP	×
0.628	NaMnP	$P4/nmm$ (129)	$P4'/n'm'm$ (129.416)	$4'/m'm'm$	PT-wP	×
0.629	NaMnAs	$P4/nmm$ (129)	$P4'/n'm'm$ (129.416)	$4'/m'm'm$	PT-wP	×
0.630	NaMnAs	$P4/nmm$ (129)	$P4'/n'm'm$ (129.416)	$4'/m'm'm$	PT-wP	×
0.631	NaMnSb	$P4/nmm$ (129)	$P4'/n'm'm$ (129.416)	$4'/m'm'm$	PT-wP	×
0.632	NaMnSb	$P4/nmm$ (129)	$P4'/n'm'm$ (129.416)	$4'/m'm'm$	PT-wP	×
0.633	$KFeS_2$	$C2/c$ (15)	$C2'/c$ (15.87)	$2'/m$	PT-wP	×
0.634	NaMnBi	$P4/nmm$ (129)	$P4'/n'm'm$ (129.416)	$4'/m'm'm$	PT-wP	×
0.635	NaMnBi	$P4/nmm$ (129)	$P4'/n'm'm$ (129.416)	$4'/m'm'm$	PT-wP	×
0.636	$RbFeS_2$	$C2/c$ (15)	$C2'/c$ (15.87)	$2'/m$	PT-wP	×
0.637	$KFeSe_2$	$C2/c$ (15)	$C2/c'$ (15.88)	$2/m'$	PT-wP	×
0.638	$RbFeSe_2$	$C2/c$ (15)	$C2/c'$ (15.88)	$2/m'$	PT-wP	×
0.639	Mn_2Au	$I4/mmm$ (139)	$Im'mm$ (71.535)	$m'mm$	PT-wP	×
0.640	Mn_2Au	$I4/mmm$ (139)	$Im'mm$ (71.535)	$m'mm$	PT-wP	×
0.641	Mn_3Ga	$I4/mmm$ (139)	$C2'/m'$ (12.62)	$2'/m'$	×	✓
0.642	$LaMnO_3$	$Pnma$ (62)	$Pn'ma'$ (62.448)	$m'm'm$	×	✓
0.643	$La_{0.95}Ca_{0.05}MnO_3$	$Pnma$ (62)	$Pn'ma'$ (62.448)	$m'm'm$	×	✓
0.644	$La_{0.95}Ba_{0.05}MnO_3$	$Pnma$ (62)	$Pn'ma'$ (62.448)	$m'm'm$	×	✓
0.645	$La_{0.95}Ba_{0.05}Mn_{0.95}Ti_{0.05}O_3$	$Pnma$ (62)	$Pn'ma'$ (62.448)	$m'm'm$	×	✓
0.646	$La_{0.90}Ba_{0.10}Mn_{0.90}Ti_{0.10}O_3$	$Pnma$ (62)	$Pn'ma'$ (62.448)	$m'm'm$	×	✓
0.647	$La_{0.875}Ba_{0.125}Mn_{0.875}Ti_{0.125}O_3$	$Pnma$ (62)	$Pn'ma'$ (62.448)	$m'm'm$	×	✓
0.648	$(Ho_{0.8}Mn_{0.2})MnO_3$	$Pnma$ (62)	$Pnm'a'$ (62.447)	$m'm'm$	×	✓
0.649	$(Ho_{0.8}Mn_{0.2})MnO_3$	$Pnma$ (62)	$Pnm'a'$ (62.447)	$m'm'm$	×	✓
0.650	$ErSi_2O_7$	$C2/m$ (12)	$C2'/m$ (12.60)	$2'/m$	PT-wP	×
0.651	$Er_3Cu_4Sn_4$	$C2/m$ (12)	C_c2/m (12.63)	$2/m1'$	×	×
0.652	$HoMnO_3$	$P6_3cm$ (185)	$P6_3'cm'$ (185.2)	$6'mm'$	BW-woP	×
0.653	$HoMn_{0.99}Fe_{0.01}O_3$	$P6_3cm$ (185)	$P6_3'cm'$ (185.2)	$6'mm'$	BW-woP	×
0.654	$HoMn_{0.95}Fe_{0.05}O_3$	$P6_3cm$ (185)	$P6_3'cm'$ (185.2)	$6'mm'$	BW-woP	×
0.655	$HoMn_{0.9}Fe_{0.1}O_3$	$P6_3cm$ (185)	$P6_3'cm'$ (185.2)	$6'mm'$	BW-woP	×
0.656	$NdMn_2Ge_2$	$I4/mmm$ (139)	$Im'm2'$ (44.231)	$m'm2'$	BW-wP	✓

Continued on next page

Suppl. Tab. XI – continued from previous page

BCS-ID	Formula	Parent	MSG	MPG	SHG type	LMO
0.657	$PrMn_2Ge_2$	$I4/mmm$ (139)	$Im'm2'$ (44.231)	$m'm2'$	BW-wP	✓
0.658	$BaCuTe_2O_6$	$P4_132$ (213)	$P4_1'32'$ (213.65)	$4'32'$	BW-woP	×
0.659	$NdMn_{0.8}Fe_{0.2}O_3$	$Pnma$ (62)	$Pn'ma'$ (62.448)	$m'm'm$	×	✓
0.660	$NdMn_{0.8}Fe_{0.2}O_3$	$Pnma$ (62)	$Pn'ma'$ (62.448)	$m'm'm$	×	✓
0.661	$(Lu_{0.6}Mn_{0.4})MnO_3$	$Pnma$ (62)	$Pnm'a'$ (62.447)	$m'm'm$	×	✓
0.662	Mn_3Sn_2	$Pnma$ (62)	$Pn'ma'$ (62.448)	$m'm'm$	×	✓
0.663	Mn_3Sn_2	$Pnma$ (62)	$Pn'ma'$ (62.448)	$m'm'm$	×	✓
0.664	Mn_3Sn_2	$Pnma$ (62)	$P2_1'/c'$ (14.79)	$2'/m'$	×	✓
0.665	$CeMnSbO$	$P4/nmm$ (129)	$P4'/n'm'm$ (129.416)	$4'/m'm'm$	PT-wP	×
0.666	$CeMnSbO$	$P4/nmm$ (129)	$Pm'mn$ (59.407)	$m'mm$	PT-wP	×
0.667	$LaMnSbO$	$P4/nmm$ (129)	$P4'/n'm'm$ (129.416)	$4'/m'm'm$	PT-wP	×
0.668	$PrMnSbO$	$P4/nmm$ (129)	$Pm'mn$ (59.407)	$m'mm$	PT-wP	×
0.669	Sr_2YbRuO_6	$P112_1/n$ (14)	$P2_1/c$ (14.75)	$2/m$	×	✓
0.670	Sr_2YbRuO_6	$P2_1/n$ (14)	$P2_1/c$ (14.75)	$2/m$	×	✓
0.671	Sr_2TmRuO_6	$P2_1/n$ (14)	$P2_1/c$ (14.75)	$2/m$	×	✓
0.672	$CaCu_3Fe_2Sb_2O_{12}$	$Pn\bar{3}$ (201)	$Pn'n'n$ (48.260)	$m'm'm$	×	✓
0.673	$MnFe_4Si_3$	$P6_3/mcm$ (193)	$P6_3/mc'm'$ (193.260)	$6/mm'm'$	×	✓
0.674	$MnFe_4Si_3$	$P6_3/mcm$ (193)	$P6_3/mc'm'$ (193.260)	$6/mm'm'$	×	✓
0.675	$MnFe_4Si_3$	$P6_3/mcm$ (193)	$P6_3/mc'm'$ (193.260)	$6/mm'm'$	×	✓
0.676	$Nd_{0.95}Sr_{0.05}CrO_3$	P (62)	$Pnma$ (62.441)	mmm	×	×
0.677	$Nd_{0.9}Sr_{0.1}CrO_3$	$Pbnm$ (62)	$Pnma$ (62.441)	mmm	×	×
0.678	$Nd_{0.85}Sr_{0.15}CrO_3$	$Pbnm$ (62)	$Pnma$ (62.441)	mmm	×	×
0.679	$TbCr_{0.5}Mn_{0.5}O_3$	$Pbnm$ (62)	$Pn'ma'$ (62.448)	$m'm'm$	×	✓
0.680	$Bi_{0.8}La_{0.2}Fe_{0.5}Mn_{0.5}O_3$	$Imma$ (74)	$Imm'a'$ (74.559)	$m'm'm$	×	✓
0.681	Ce_4Sb_3	$I\bar{4}3d$ (220)	$I\bar{4}'2d'$ (122.336)	$\bar{4}'2m'$	BW-woP	×
0.682	Ca_2FeOsO_6	$P2_1/n$ (14)	$P2_1'/c'$ (14.79)	$2'/m'$	×	✓
0.683	$SrCaFeOsO_6$	$P2_1/n$ (14)	$P2_1'/c'$ (14.79)	$2'/m'$	×	✓
0.684	$TbPt$	$Pnma$ (62)	$Pn'm'a$ (62.446)	$m'm'm$	×	✓
0.685	$ErPt$	$Pnma$ (62)	$Pnm'a'$ (62.447)	$m'm'm$	×	✓
0.686	$HoPt$	$Pnma$ (62)	$Pnm'a'$ (62.447)	$m'm'm$	×	✓
0.687	$DyPt$	$Pnma$ (62)	$Pn'm'a$ (62.446)	$m'm'm$	×	✓
0.688	$TmPt$	$Pnma$ (62)	$Pnm'a'$ (62.447)	$m'm'm$	×	✓
0.689	$PrPt$	$Cmcm$ (63)	$Cm'c'm$ (63.462)	$m'm'm$	×	✓
0.690	$NdPt$	$Cmcm$ (63)	$C2'/c'$ (15.89)	$2'/m'$	×	✓
0.691	$CaCo_{1.86}As_2$	$I4/mmm$ (139)	P_I4/nnc (126.386)	$4/mmm1'$	×	×
0.692	Ba_4Ru_3O10	$Cmce$ (64)	$Cm'ca$ (64.471)	$m'mm$	PT-wP	×
0.693	Ba_4Ru_3O10	$Cmce$ (64)	$Cmc'a$ (64.472)	$m'mm$	PT-wP	×
0.694	Bi_2CuO_4	$P4/ncc$ (130)	$P4/n'c'c'$ (130.431)	$4/m'm'm'$	PT-wP	×
0.695	Bi_2CuO_4	$P4/ncc$ (130)	$Pc'cn$ (56.367)	$m'mm$	PT-wP	×
0.696	$SmCrO_3$	$Pbnm$ (62)	$Pn'ma'$ (62.448)	$m'm'm$	×	✓
0.697	$SmCrO_3$	$Pbnm$ (62)	$Pn'm'a$ (62.446)	$m'm'm$	×	✓
0.698	$SmCrO_3$	$Pbnm$ (62)	$Pbn'm'$ (62.446)	$m'm'm$	×	✓
0.699	$LiMn_6Sn_6$	$P6/mmm$ (191)	$Cmm'm'$ (65.486)	$m'm'm$	×	✓
0.700	$TbMn_6Sn_6$	$P6/mmm$ (191)	$P6/mm'm'$ (191.240)	$6/mm'm'$	×	✓
0.701	$TbMn_6Sn_6$	$P6/mmm$ (191)	$P6/mm'm'$ (191.240)	$6/mm'm'$	×	✓
0.702	$TbMn_6Sn_6$	$P6/mmm$ (191)	$C2'/m'$ (12.62)	$2'/m'$	×	✓
0.703	$HoMn_6Sn_6$	$P6/mmm$ (191)	$C2'/m'$ (12.62)	$2'/m'$	×	✓
0.704	$HoMn_6Sn_6$	$P6/mmm$ (191)	$C2'/m'$ (12.62)	$2'/m'$	×	✓
0.705	$HoMn_6Sn_6$	$P6/mmm$ (191)	$Cmm'm'$ (65.486)	$m'm'm$	×	✓
0.706	$Tb_2Ir_3Ga_9$	$Cmcm$ (63)	$Cm'cm'$ (63.464)	$m'm'm$	×	✓
0.707	$Tb_2Ir_3Ga_9$	$Cmcm$ (63)	$Cm'cm'$ (63.464)	$m'm'm$	×	✓

Continued on next page

Suppl. Tab. XI – continued from previous page

BCS-ID	Formula	Parent	MSG	MPG	SHG type	LMO
0.708	$CrNb_4S_8$	$P6_3/mmc$ (194)	$P6_3'/m'm'c$ (194.268)	$6'/m'mm'$	×	×
0.709	$MnNb_4S_8$	$P6_3/mmc$ (194)	$Cmc'm'$ (63.463)	$m'm'm$	×	✓
0.710	$MnNb_3S_6$	$P6_322$ (182)	$C22'2_1'$ (20.34)	$2'2'2$	BW-woP	✓
0.711	$MnTa_4S_8$	$P6_3/mmc$ (194)	$Cmc'm'$ (63.463)	$m'm'm$	×	✓
0.712	VNb_3S_6	$P6_322$ (182)	$C2'2'2_1$ (20.33)	$2'2'2$	BW-woP	✓
0.713	$NiFe_2O_4$	$Fd\bar{3}m$ (227)	$I4_1/am'd'$ (141.557)	$4/mm'm'$	×	✓
0.714	$Li_2Ni(SO_4)_2$	$P2_1/c$ (14)	$P2_1/c$ (14.75)	$2/m$	×	✓
0.715	$HoCrWO_6$	$Pna2_1$ (33)	$Pna2_1$ (33.144)	$mm2$	O-woP	×
0.716	$HoCrWO_6$	$Pna2_1$ (33)	$Pna2_1$ (33.144)	$mm2$	O-woP	×
0.717	$Pr_{0.5}Sr_{0.4}Ba_{0.1}CoO_3$	$Imma$ (74)	$Im'm'a$ (74.558)	$m'm'm$	×	✓
0.718	$Pr_{0.5}Sr_{0.4}Ba_{0.1}CoO_3$	$I4/mcm$ (140)	$Fm'm'm$ (69.524)	$m'm'm$	×	✓
0.719	$Yb_{0.42}Sc_{0.58}FeO_3$	$P6_3cm$ (185)	$P6_3c'm'$ (185.201)	$6m'm'$	BW-woP	✓
0.720	$Yb_{0.42}Sc_{0.58}FeO_3$	$P6_3cm$ (185)	$P6_3$ (173.129)	6	O-woP	✓
0.721	$Yb_{0.42}Sc_{0.58}FeO_3$	$P6_3cm$ (185)	$P6_3$ (173.129)	6	O-woP	✓
0.722	$Mn_4Nb_2O_9$	Cc (9)	Cc (9.37)	m	O-woP	✓
0.723	$YbCl_3$	$C2/m$ (12)	$C2'/m$ (12.60)	$2'/m$	PT-wP	×
0.724	$BaCoSiO_4$	$P6_3$ (173)	$P6_3$ (173.129)	6	O-woP	✓
0.725	Ce_5TeO_8	$Fd\bar{3}m$ (227)	$I4_1/am'd'$ (141.557)	$4/mm'm'$	×	✓
0.726	$CsMn_2F_6$	$Pnma$ (62)	$Pnm'a'$ (62.447)	$m'm'm$	×	✓
0.727	$CsMn_2F_6$	$Pnma$ (62)	$P2_1/c$ (14.75)	$2/m$	×	✓
0.728	MoP_3SiO_{11}	$R\bar{3}c$ (167)	$C2/c'$ (15.88)	$2/m'$	PT-wP	×
0.729	$ErNi_4B$	$P6/mmm$ (191)	$P6/mm'm'$ (191.240)	$6/mm'm'$	×	✓
0.730	$TbNi_4B$	$P6/mmm$ (191)	$C2'/m'$ (12.62)	$2'/m'$	×	✓
0.731	$HoNi_4B$	$P6/mmm$ (191)	$C2'/m'$ (12.62)	$2'/m'$	×	✓
0.732	$SrRuO_3$	$Pnma$ (62)	$Pn'm'a$ (62.446)	$m'm'm$	×	✓
0.733	$AgRuO_3$	$R\bar{3}c$ (167)	$R\bar{3}'c'$ (167.106)	$\bar{3}'m'$	PT-wP	×
0.734	$Mn_3Ta_2O_8$	$I4_1/a$ (88)	$C2'/c$ (15.87)	$2'/m$	PT-wP	×
0.735	$LaBaMn_2O_5$	$P4/nmm$ (129)	$P4/nm'm'$ (129.417)	$4/mm'm'$	×	✓
0.736	$LaBaMn_2O_6$	$Pm\bar{3}m$ (221)	$P4/mm'm'$ (123.345)	$4/mm'm'$	×	✓
0.737	$LaBaMn_2O_6$	$P4/mmm$ (123)	$P4/mm'm'$ (123.345)	$4/mm'm'$	×	✓
0.738	$LaBaMn_2O_6$	$P4/mmm$ (123)	$P4/mm'm'$ (123.345)	$4/mm'm'$	×	✓
0.739	$YBaMn_2O_5$	$P4/nmm$ (129)	$P4/nm'm'$ (129.417)	$4/mm'm'$	×	✓
0.740	$Dy_3Ga_5O_{12}$	$Ia\bar{3}d$ (230)	$Ia\bar{3}d'$ (230.148)	$m\bar{3}m'$	×	×
0.741	$Er_3Ga_5O_{12}$	$Ia\bar{3}d$ (230)	$Ia\bar{3}d'$ (230.148)	$m\bar{3}m'$	×	×
0.742	$Tb_3Ga_5O_{12}$	$Ia\bar{3}d$ (230)	$Ia\bar{3}d'$ (230.148)	$m\bar{3}m'$	×	×
0.743	$Ho_3Al_5O_{12}$	$Ia\bar{3}d$ (230)	$Ia\bar{3}d'$ (230.148)	$m\bar{3}m'$	×	×
0.744	$Tb_3Al_5O_{12}$	$Ia\bar{3}d$ (230)	$Ia\bar{3}d'$ (230.148)	$m\bar{3}m'$	×	×
0.745	$Ho_3Ga_5O_{12}$	$Ia\bar{3}d$ (230)	$Ia\bar{3}d'$ (230.148)	$m\bar{3}m'$	×	×
0.746	$Tb_3Ga_5O_{12}$	$Ia\bar{3}d$ (230)	$Ia\bar{3}d'$ (230.148)	$m\bar{3}m'$	×	×
0.747	$Ba_3CoIr_2O_9$	$C2/c$ (15)	$C2/c$ (15.85)	$2/m$	×	✓
0.748	$Ba_3NiRu_2O_9$	$P6_3/mmc$ (194)	$P6_3'/m'm'c$ (194.268)	$6'/m'mm'$	×	×
0.749	$Ba_3CoRu_2O_9$	$Cmcm$ (63)	P_Bnma (62.454)	$mmm1'$	×	×
0.750	$Ba_3CoRu_2O_9$	$P6_3/mmc$ (194)	P_Bnma (62.454)	$mmm1'$	×	×
0.751	$Ca_2YZr_2Fe_3O_{12}$	$Ia\bar{3}d$ (230)	$R\bar{3}'c$ (167.105)	$\bar{3}'m$	PT-wP	×
0.752	$Ca_2YZr_2Fe_3O_{12}$	$Ia\bar{3}d$ (230)	$R\bar{3}'c$ (167.105)	$\bar{3}'m$	PT-wP	×
0.753	$Ca_2LaZr_2Fe_3O_{12}$	$Ia\bar{3}d$ (230)	$R\bar{3}'c$ (167.105)	$\bar{3}'m$	PT-wP	×
0.754	$Ca_2LaZr_2Fe_3O_{12}$	$Ia\bar{3}d$ (230)	$R\bar{3}'c$ (167.105)	$\bar{3}'m$	PT-wP	×
0.755	$Mn_2SeO_3F_2$	$Pnma$ (62)	$Pn'ma'$ (62.448)	$m'm'm$	×	✓
0.756	GaV_4S_8	$R3m$ (160)	$R3m'$ (160.67)	$3m'$	BW-woP	✓
0.757	$CeFeO_3$	$Pbnm$ (62)	$Pn'ma'$ (62.448)	$m'm'm$	×	✓
0.758	$CeFeO_3$	$Pbnm$ (62)	$Pnma$ (62.441)	mmm	×	×

Continued on next page

Suppl. Tab. XI – continued from previous page

BCS-ID	Formula	Parent	MSG	MPG	SHG type	LMO
0.759	$CeFeO_3$	$Pbnm$ (62)	$Pnma$ (62.441)	mmm	×	×
0.760	$FeOHSO_4$	$C2/c$ (15)	$C2'/c'$ (15.89)	$2'/m'$	×	✓
0.761	$SrFe_2Se_2O$	$Pmmn$ (59)	$Pm'm'n'$ (59.411)	$m'm'm'$	PT-wP	×
0.762	$SrFe_2S_2O$	$Pmmn$ (59)	$Pm'm'n'$ (59.411)	$m'm'm'$	PT-wP	×
0.763	$Mn_5(PO_4)_2(PO_3(OH))_2(HOH)_4$	$C2/c$ (15)	$C2'/c'$ (15.89)	$2'/m'$	×	✓
0.764	$Mn_5(PO_4)_2(PO_3(OH))_2(HOH)_4$	$C2/c$ (15)	$C2'/c'$ (15.89)	$2'/m'$	×	✓
0.765	$Mn_5(PO_4)_2(PO_3(OH))_2(HOH)_4$	$C2/c$ (15)	$C2'/c'$ (15.89)	$2'/m'$	×	✓
0.766	$YbMnSb_2$	$P4/nmm$ (129)	$P4'/n'm'm$ (129.416)	$4'/m'm'm$	PT-wP	×
0.767	$SrMnSb_2$	$Pnma$ (62)	$Pn'ma'$ (62.448)	$m'm'm$	×	✓
0.768	$SrMnSb_2$	$Pnma$ (62)	$Pn'a'2_1$ (33.148)	$m'm'2$	BW-wP	✓
0.769	$YbMnBi_2$	$P4/nmm$ (129)	$P4'/n'm'm$ (129.416)	$4'/m'm'm$	PT-wP	×
0.770	$Fe_2Co_2Nb_2O_9$	$P\bar{3}1c$ (165)	$C2/c'$ (15.88)	$2/m'$	PT-wP	×
0.771	$PrMnSi_2$	$Cmcm$ (63)	$Cm'cm'$ (63.464)	$m'm'm$	×	✓
0.772	$PrMnSi_2$	$Cmcm$ (63)	$Cm'cm'$ (63.464)	$m'm'm$	×	✓
0.773	$NdMnSi_2$	$Cmcm$ (63)	$C2'/m'$ (12.62)	$2'/m'$	×	✓
0.774	$NdMnSi_2$	$Cmcm$ (63)	$Cm'cm'$ (63.464)	$m'm'm$	×	✓
0.775	$NdMnSi_2$	$Cmcm$ (63)	$Cm'cm'$ (63.464)	$m'm'm$	×	✓
0.776	$CeMnSi_2$	$Cmcm$ (63)	$Cm'cm'$ (63.464)	$m'm'm$	×	✓
0.777	$CeMnSi_2$	$Cmcm$ (63)	$Cm'cm'$ (63.464)	$m'm'm$	×	✓
0.778	$LaMnSi_2$	$Cmcm$ (63)	$Cm'cm'$ (63.464)	$m'm'm$	×	✓
0.779	$LaMnSi_2$	$Cmcm$ (63)	$Cm'cm'$ (63.464)	$m'm'm$	×	✓
0.780	$LaMnSi_2$	$Cmcm$ (63)	$Cm'cm'$ (63.464)	$m'm'm$	×	✓
0.781	$CeMnSi_2$	$Cmcm$ (63)	$Cm'cm'$ (63.464)	$m'm'm$	×	✓
0.782	$NdScO_3$	$Pbnm$ (62)	$Pnm'a$ (62.444)	$m'mm$	PT-wP	×
0.783	$NdInO_3$	$Pbnm$ (62)	$Pnm'a$ (62.444)	$m'mm$	PT-wP	×
0.784	$NdCoO_3$	$Pbnm$ (62)	$Pnma$ (62.441)	mmm	×	×
0.785	$NdVO_3$	$Pbnm$ (62)	$P2_1'/m'$ (11.54)	$2'/m'$	×	✓
0.786	$NdVO_3$	$Pbnm$ (62)	$P2_1'/m'$ (11.54)	$2'/m'$	×	✓
0.787	YVO_3	$Pbnm$ (62)	$Pn'm'a$ (62.446)	$m'm'm$	×	✓
0.788	YVO_3	$P2_1/b11$ (14)	$P\bar{1}$ (2.4)	$\bar{1}$	×	✓
0.789	$CeCuSi$	$P6_3/mmc$ (194)	$Cmc'm'$ (63.463)	$m'm'm$	×	✓
0.790	Sr_2DyRuO_6	$P2_1/n$ (14)	$P2_1'/c'$ (14.79)	$2'/m'$	×	✓
0.791	Sr_2TbRuO_6	$P2_1/n$ (14)	$P2_1/c$ (14.75)	$2/m$	×	✓
0.792	Sr_2HoRuO_6	$P2_1/n$ (14)	$P2_1/c$ (14.75)	$2/m$	×	✓
0.793	Sr_2HoRuO_6	$P2_1/n$ (14)	$P2_1/c$ (14.75)	$2/m$	×	✓
0.794	Sr_2HoRuO_6	$P2_1/n$ (14)	$P2_1/c$ (14.75)	$2/m$	×	✓
0.795	Sr_2YRuO_6	$P2_1/c$ (14)	$P2_1/c$ (14.75)	$2/m$	×	✓
0.796	Ca_2NiOsO_6	$P2_1/n$ (14)	$P2_1'/c'$ (14.79)	$2'/m'$	×	✓
0.797	$SmBaMn_2O_5$	$P4/nmm$ (129)	$P4/nm'm'$ (129.417)	$4/mm'm'$	×	✓
0.798	$MnPd_2$	$Pnma$ (62)	$Pnma'$ (62.445)	$m'mm$	PT-wP	×
0.799	$Sr_2Co_2O_5$	$Ima2$ (46)	P_Inc2 (30.122)	$mm21'$	G-woP	×
0.800	$MnTe$	$P6_3/mmc$ (194)	$Cmcm$ (63.457)	mmm	×	×
0.801	$Tl_3Fe_2S_4$	$Pnma$ (62)	$Pnma'$ (62.445)	$m'mm$	PT-wP	×
0.802	$CuFeS_2$	$I\bar{4}2d$ (122)	$I\bar{4}2d$ (122.333)	$\bar{4}2m$	O-woP	×
0.803	$NbMnP$	$Pnma$ (62)	$Pm'n2_1'$ (31.125)	$m'm2'$	BW-wP	✓
0.804	MoP_3SiO_{11}	$R\bar{3}c$ (167)	$C2/c'$ (15.88)	$2/m'$	PT-wP	×
0.805	$DyBaCuO_5$	$Pnma$ (62)	$Pnm'a$ (62.444)	$mm'm$	PT-wP	×
0.806	$Fe_2Se_2O_7$	$Pccn$ (56)	$Pc'cn$ (56.367)	$m'mm$	PT-wP	×
0.807	$Fe_2Se_2O_7$	$Pccn$ (56)	$Pc'cn$ (56.367)	$m'mm$	PT-wP	×
0.808	$Fe_2Se_2O_7$	$Pccn$ (56)	$Pc'cn$ (56.367)	$m'mm$	PT-wP	×
0.809	Fe_2WO_6	$P2_1/c$ (14)	$P2_1/c'$ (14.78)	$2/m'$	PT-wP	×

Continued on next page

Suppl. Tab. XI – continued from previous page

BCS-ID	Formula	Parent	MSG	MPG	SHG type	LMO
0.810	Fe_2WO_6	$Pbcn$ (60)	$Pbc'n'$ (60.423)	$m'm'm$	×	✓
0.811	Fe_2WO_6	$Pbcn$ (60)	$Pbc'n'$ (60.423)	$m'm'm$	×	✓
0.812	Fe_2WO_6	$Pbcn$ (60)	$Pn'c2'$ (30.113)	$m'm2'$	BW-wP	✓
0.813	Fe_2WO_6	$Pbcn$ (60)	$Pbc'n'$ (60.423)	$m'm'm$	×	✓
0.814	Fe_2WO_6	$Pbcn$ (60)	$Pb'cn$ (60.419)	$m'mm$	PT-wP	×
0.815	$MnNb_2O_6$	$Pbcn$ (60)	$Pb'cn$ (60.419)	$m'mm$	PT-wP	×
0.816	$MnTa_2O_6$	$Pbcn$ (60)	$Pb'cn$ (60.419)	$m'mm$	PT-wP	×
0.817	$Mn(Nb_{0.5}Ta_{0.5})_2O_6$	$Pbcn$ (60)	$Pb'cn$ (60.419)	$m'mm$	PT-wP	×
0.818	$MnTa_2O_6$	$Pbcn$ (60)	$Pb'cn$ (60.419)	$m'mm$	PT-wP	×
0.819	$MnNb_2O_6$	$Pbcn$ (60)	$Pb'cn$ (60.419)	$m'mm$	PT-wP	×
0.820	$Bi_{0.85}Ca_{0.15}Fe_{0.55}Mn_{0.45}O_3$	$Pnma$ (62)	$Pn'm'a$ (62.446)	$m'm'm$	×	✓
0.821	$SrGd_2O_4$	$Pnma$ (62)	$Pnma'$ (62.445)	$m'mm$	PT-wP	×
0.822	Nd_2ScNbO_7	$Fd\bar{3}m$ (227)	$Fd\bar{3}m'$ (227.131)	$m\bar{3}m'$	×	×
0.823	Sr_2MnGaO_5	$Ima2$ (46)	$Im'a2'$ (46.243)	$m'm2'$	BW-woP	✓
0.824	$Sr_2MnGaO_{5.5}$	$P4/mmm$ (123)	P_C4/mbm (127.397)	$4/mmm1'$	×	×
0.825	Ca_2MnGaO_5	$Pnma$ (62)	$Pnm'a'$ (62.447)	$m'm'm$	×	✓
0.826	$MnTeLi0.00_3$	$P6_3/mmc$ (194)	$C2'/m'$ (12.62)	$2'/m'$	×	✓
0.827	Na_2MnPO_4F	$P2_1/c$ (14)	$P2_1/c'$ (14.78)	$2/m'$	PT-wP	×
0.828	Na_2MnPO_4F	$P2_1/n$ (14)	$P2_1/c'$ (14.78)	$2/m'$	PT-wP	×
0.829	Na_2MnPO_4F	$P2_1/n$ (14)	$P2_1/c'$ (14.78)	$2/m'$	PT-wP	×
0.830	Na_2MnPO_4F	$P2_1/n$ (14)	$P2_1/c'$ (14.78)	$2/m'$	PT-wP	×
0.831	$BaCaFe_4O_7$	$Pbn2_1$ (33)	$Pn'a'2_1$ (33.148)	$m'm'2$	BW-woP	✓
0.832	CeAuGe	$P6_3mc$ (186)	$Cmc'2_1'$ (36.175)	$m'm2'$	BW-woP	✓
0.833	CeCuGe	$P6_3/mmc$ (194)	$Cmc'm'$ (63.463)	$m'm'm$	×	✓
0.834	$CrSbSe_3$	$Pnma$ (62)	$Pnm'a'$ (62.447)	$m'm'm$	×	✓
0.835	$Dy_5Pd_2In_4$	$PPbam$ (55)	$Pb'a'm$ (55.357)	$m'm'm$	×	✓
1.0.1	Ag_2CrO_2	$P\bar{3}m1$ (164)	$C2'/m$ (12.60)	$2'/m$	PT-wP	×
1.0.2	$URu_{0.96}Rh_{0.04}Si_2$	$I4/mmm$ (139)	$Im'm'm$ (71.536)	$m'm'm$	×	✓
1.0.3	$CsCoBr_3$	$P6_3/mmc$ (194)	$Cm'c2_1'$ (36.174)	$m'm2'$	BW-wP	✓
1.0.4	$CsNiCl_3$	$P6_3/mmc$ (194)	$C22'2_1'$ (20.34)	$2'2'2$	BW-wP	✓
1.0.5	Sr_3CoIrO_6	$R\bar{3}c$ (167)	$P\bar{3}c'1$ (165.95)	$\bar{3}m'$	×	✓
1.0.6	CoV_2O_6	$C2/m$ (12)	$C2'/m'$ (12.62)	$2'/m'$	×	✓
1.0.7	$LuFe_2O_4$	$R\bar{3}m$ (166)	$C2'/m'$ (12.62)	$2'/m'$	×	✓
1.0.8	$Ba_3MnNb_2O_9$	$P\bar{3}m1$ (164)	$P31m$ (157.53)	$3m$	O-wP	×
1.0.9	$CsCoCl_3$	$P6_3/mmc$ (194)	$P6_3'/m'cm'$ (193.259)	$6'/m'mm'$	×	×
1.0.10	Sr_3NiIrO_6	$R\bar{3}c$ (167)	$P\bar{3}c'1$ (165.95)	$\bar{3}m'$	×	✓
1.0.11	$CeCoGe_3$	$I4mm$ (107)	$I4m'm'$ (107.231)	$4m'm'$	BW-woP	✓
1.0.12	UAu_2Si_2	$I4/mmm$ (139)	$Im'm'm$ (71.536)	$m'm'm$	×	✓
1.0.13	FeI_2	$P\bar{3}m1$ (164)	$C2'/m'$ (12.62)	$2'/m'$	×	✓
1.0.14	$CsFeCl_3$	$P6_3/mmc$ (194)	$P\bar{6}'2'm$ (189.223)	$\bar{6}'m2'$	BW-wP	×
1.0.15	$La_{0.33}Sr_{0.67}FeO_3$	$R\bar{3}c$ (167)	$P322_1$ (154.41)	32	O-wP	×
1.0.16	$La_{0.33}Sr_{0.67}FeO_3$	$R\bar{3}c$ (167)	$C2/c$ (15.85)	$2/m$	×	✓
1.0.17	$CaBaCo_2Fe_2O_7$	$P6_3mc$ (186)	$P31m'$ (157.55)	$3m'$	BW-woP	✓
1.0.18	$Cs_2MnU_3F_{16}$	$P6_3/mmc$ (194)	$P6_3/mc'm'$ (193.260)	$6/mm'm'$	×	✓
1.0.19	$Cs_2CoU_3F_{16}$	$P6_3/mmc$ (194)	$P6_3/mc'm'$ (193.260)	$6/mm'm'$	×	✓
1.0.20	$Cs_2NiU_3F_{16}$	$P6_3/mmc$ (194)	$P6_3/mc'm'$ (193.260)	$6/mm'm'$	×	✓
1.0.21	$K_2Mn_3(VO_4)_2CO_3$	$P6_3/m$ (176)	$P6_3'/m$ (176.145)	$6'/m$	PT-wP	×
1.0.22	$K_2Mn_3(VO_4)_2CO_3$	$P6_3/m$ (176)	$P2_1'$ (4.9)	$2'$	BW-wP	✓
1.0.23	$Dy_3Ru_4Al_{12}$	$P6_3/mmc$ (194)	$C2'/m'$ (12.62)	$2'/m'$	×	✓
1.0.24	$ThMn_2$	$P6_3/mmc$ (194)	$P\bar{6}'2'm$ (189.223)	$\bar{6}'m2'$	BW-wP	×
1.0.25	$CaBaCo_3FeO_7$	$Pna2_1$ (33)	$Pn'a'2_1$ (33.148)	$m'm'2$	BW-woP	✓

Continued on next page

Suppl. Tab. XI – continued from previous page

BCS-ID	Formula	Parent	MSG	MPG	SHG type	LMO
1.0.26	$RbCoBr_3$	$P6_3/mmc$ (194)	$P6_3'/m'cm'$ (193.259)	$6'/m'mm'$	×	×
1.0.27	Li_2MnTeO_6	$P\bar{3}1c$ (163)	$P\bar{3}c1$ (165.91)	$\bar{3}m$	×	×
1.0.28	$Tb(DCO_2)_3$	$R3m$ (160)	$P3m'1$ (156.51)	$3m'$	BW-woP	✓
1.0.29	$CeIrGe_3$	$I4mm$ (107)	$I4m'm'$ (107.231)	$4m'm'$	BW-woP	✓
1.0.30	$LaCa_2Fe_3O_9$	$Pnma$ (62)	$Pmn2_1$ (31.123)	$mm2$	O-wP	×
1.0.31	$EuIn_2As_2$	$P6_3/mmc$ (194)	$C2'2'2_1$ (20.33)	$2'2'2$	BW-wP	✓
1.0.32	$EuIn_2As_2$	$P6_3/mmc$ (194)	$P612'2'$ (178.159)	$62'2'$	BW-wP	✓
1.0.33	FeF_3	$P6/mmm$ (191)	$P6_3/m$ (176.143)	$6/m$	×	✓
1.0.34	$RbNiCl_3$	$P6_3/mmc$ (194)	$Cm'c2_1'$ (36.174)	$m'm2'$	BW-wP	✓
1.0.35	$CsMnBr_3$	$P6_3/mmc$ (194)	$P\bar{6}2'm'$ (189.225)	$\bar{6}m'2'$	BW-wP	✓
1.0.36	$CsMnI_3$	$P6_3/mmc$ (194)	$Cm'c2_1'$ (36.174)	$m'm2'$	BW-wP	✓
1.0.37	$CsMnI_3$	$P6_3/mmc$ (194)	$Cm'c2_1'$ (36.174)	$m'm2'$	BW-wP	✓
1.0.38	$CsCoCl_3$	$P6_3/mmc$ (194)	$P6_3'/m'cm'$ (193.259)	$6'/m'mm'$	×	×
1.0.39	$BaMnO_3$	$P6_3/mmc$ (194)	$P6_3'/m'cm'$ (193.259)	$6'/m'mm'$	×	×
1.0.40	$RbFeCl_3$	$P6_3/mmc$ (194)	$P\bar{6}'2m'$ (189.224)	$\bar{6}'m'2$	BW-wP	×
1.0.41	$RbNiCl_3$	$P6_3/mmc$ (194)	$C22'2_1'$ (20.34)	$2'2'2$	BW-wP	✓
1.0.42	$CsNiCl_3$	$P6_3/mmc$ (194)	$C22'2_1'$ (20.34)	$2'2'2$	BW-wP	✓
1.0.43	UPd_2Si_2	$I4/mmm$ (139)	$I4/mm'm'$ (139.537)	$4/mm'm'$	×	✓
1.0.44	$Ba_3CoSb_2O_9$	$P6_3/mmc$ (194)	$Cm'c2_1'$ (36.174)	$m'm2'$	BW-wP	✓
1.0.45	$Ba_3CoSb_2O_9$	$P6_3/mmc$ (194)	$P\bar{6}2m$ (189.221)	$\bar{6}m2$	O-wP	×
1.0.46	$Ba_3MnSb_2O_9$	$C2/c$ (15)	$C2$ (5.13)	2	O-wP	✓
1.0.47	$MnSe_2$	$Pa\bar{3}$ (205)	$Pbca$ (61.433)	mmm	×	×
1.0.48	$MnSe_2$	$Pa\bar{3}$ (205)	$Pca'2_1'$ (29.102)	$m'm2'$	BW-wP	✓
1.0.49	$BaCoSiO_4$	$P6_3$ (173)	$P6_3$ (173.129)	6	O-woP	✓
1.0.50	$CoGeO_3$	$C2/c$ (15)	$C2'/c'$ (15.89)	$2'/m'$	×	✓
1.0.51	Na_2MnTeO_6	$P\bar{3}1c$ (163)	$R\bar{3}'c'$ (167.106)	$\bar{3}'m'$	PT-wP	×
1.0.52	$Tb_{14}Ag_{51}$	$P6/m$ (175)	$P\bar{6}'$ (174.135)	$\bar{6}'$	BW-wP	×
1.1	Mn_3O_4	$Pbcm$ (57)	P_cnma (62.452)	$mmm1'$	×	×
1.2	$CuSe_2O_5$	$C2/c$ (15)	P_c2_1/c (14.84)	$2/m1'$	×	×
1.3	Sr_2IrO_4	$I4_1/acd$ (142)	P_Icca (54.352)	$mmm1'$	×	×
1.4	$YBa_2Cu_3O_{6+d}$	$P4/mmm$ (123)	C_ammm (65.489)	$mmm1'$	×	×
1.5	$YBa_2Cu_3O_{6+d}$	$P4/mmm$ (123)	F_Smmm (69.526)	$mmm1'$	×	×
1.6	NiO	$Fm\bar{3}m$ (225)	C_c2/c (15.90)	$2/m1'$	×	×
1.7	$NdFe_3B_4O_{12}$	$R32$ (155)	C_c2 (5.16)	$21'$	G-woP	×
1.8	$CeRu_2Al_{10}$	$Cmcm$ (63)	P_Cbcm (57.391)	$mmm1'$	×	×
1.9	Li_2VOSiO_4	$P4/nmm$ (129)	P_Abcm (57.389)	$mmm1'$	×	×
1.1	Na_2IrO_3	$C2/m$ (12)	C_c2/m (12.63)	$2/m1'$	×	×
1.11	$Bi_4Fe_5O_{13}F$	$P4_2/mbc$ (135)	P_C42/n (86.73)	$4/m1'$	×	×
1.12	$BaNd_{0.9}Y_{0.1}MoO_6$	$I4/m$ (87)	P_I4/m (83.50)	$4/m1'$	×	×
1.13	$Ba_3Nb_2NiO_9$	$P\bar{3}m1$ (164)	P_c31c (159.64)	$3m1'$	G-wP	×
1.14	Ho_2BaNiO_5	$Immm$ (71)	C_c2/c (15.90)	$2/m1'$	×	×
1.15	Er_2BaNiO_5	$Immm$ (71)	C_c2/c (15.90)	$2/m1'$	×	×
1.16	$BaFe_2As_2$	$I4/mmm$ (139)	C_Amca (64.480)	$mmm1'$	×	×
1.17	CoV_2O_6-alpha	$C2/m$ (12)	C_c2/c (15.90)	$2/m1'$	×	×
1.18	MnS_2	$Pa\bar{3}$ (205)	P_bca2_1 (29.105)	$mm21'$	G-wP	×
1.19	$PrMn_2O_5$	$Pbam$ (55)	P_aca2_1 (29.104)	$mm21'$	G-wP	×
1.20	$HoMnO_3$	$Pnma$ (62)	P_bmn2_1 (31.129)	$mm21'$	G-wP	×
1.21	$DyCo_2Si_2$	$I4/mmm$ (139)	P_I4/mnc (128.410)	$4/mmm1'$	×	×
1.22	$DyCu_2Si_2$	$I4/mmm$ (139)	C_c2/m (12.63)	$2/m1'$	×	×
1.23	La_2CuO_4	$Cmce$ (64)	P_Accn (56.374)	$mmm1'$	×	×
1.24	ZnV_2O_4	$I4_1/amd$ (141)	$P_I4_32_12$ (96.150)	$4221'$	G-wP	×

Continued on next page

Suppl. Tab. XI – continued from previous page

BCS-ID	Formula	Parent	MSG	MPG	SHG type	LMO
1.25	$KFe_3(OH)_6(SO_4)_2$	$R\bar{3}m$ (166)	$R_I\bar{3}c$ (167.108)	$\bar{3}m1'$	×	×
1.26	$CsFe_2Se_3$	$Cmcm$ (63)	P_c2_1/c (14.82)	$2/m1'$	×	×
1.27	$TaFe_{1+y}Te_3$	$P2_1/m$ (11)	P_c2_1/c (14.82)	$2/m1'$	×	×
1.28	CrN	$Fm\bar{3}m$ (225)	P_anma (62.450)	$mmm1'$	×	×
1.29	$LaSrFeO_4$	$I4/mmm$ (139)	C_Amca (64.480)	$mmm1'$	×	×
1.30	$BaCo_2V_2O_8$	$I4_1/acd$ (142)	P_Icca (54.352)	$mmm1'$	×	×
1.31	MnO	$Fm\bar{3}m$ (225)	C_c2/c (15.90)	$2/m1'$	×	×
1.32	Lu_2MnCoO_6	$P2_1/n$ (14)	P_a2_1 (4.10)	$21'$	G-wP	×
1.33	ErAuGe	$P6_3mc$ (186)	P_Cna2_1 (33.154)	$mm21'$	G-woP	×
1.34	HoAuGe	$P6_3mc$ (186)	P_Cna2_1 (33.154)	$mm21'$	G-woP	×
1.35	$LiErF_4$	$I4_1/a$ (88)	P_C2_1/c (14.84)	$2/m1'$	×	×
1.36	Dy_2BaNiO_5	$Immm$ (71)	C_c2/c (15.90)	$2/m1'$	×	×
1.37	VOCl	$Pmmn$ (59)	C_a2/c (15.91)	$2/m1'$	×	×
1.38	Nd_2NaOsO_6	$P2_1/n$ (14)	$P_S\bar{1}$ (2.7)	$\bar{1}1'$	×	×
1.39	$LiFeGe_2O_6$	$P2_1/c$ (14)	P_a2_1/c (14.80)	$2/m1'$	×	×
1.40	$SrNdFeO_4$	$I4/mmm$ (139)	C_Accm (66.5)	$mmm1'$	×	×
1.41	$SrNdFeO_4$	$I4/mmm$ (139)	C_Amca (64.480)	$mmm1'$	×	×
1.42	La_2NiO_4	$Bmeb$ (64)	P_Cmna (53.335)	$mmm1'$	×	×
1.43	$PrNiO_3$	$Pbnm$ (62)	C_amc2_1 (36.178)	$mm21'$	G-wP	×
1.44	$NdNiO_3$	$Pbnm$ (62)	C_amc2_1 (36.178)	$mm21'$	G-wP	×
1.45	$NdNiO_3$	$Pbnm$ (62)	C_amc2_1 (36.178)	$mm21'$	G-wP	×
1.46	Sr_2FeOsO_6	$I4/m$ (87)	P_c4/n (85.64)	$4/m1'$	×	×
1.47	Sr_2FeOsO_6	$I4/m$ (87)	P_I4/m (83.50)	$4/m1'$	×	×
1.48	$HoNiO_3$	$P2_1/n$ (14)	P_a2_1 (4.10)	$21'$	G-wP	×
1.49	Ag_2NiO_2	$C2/m$ (12)	C_c2/c (15.90)	$2/m1'$	×	×
1.50	$AgNiO_2$	$P6_322$ (182)	$P_B2_12_12$ (18.22)	$2221'$	G-woP	×
1.51	Cs_2CoCl_4	$Pnma$ (62)	P_a2_1 (4.10)	$21'$	G-wP	×
1.52	$CaFe_2As_2$	$I4/mmm$ (139)	C_Amca (64.480)	$mmm1'$	×	×
1.53	Er_2BaNiO_5	$Immm$ (71)	C_c2/c (15.90)	$2/m1'$	×	×
1.54	$GdMn_2O_5$	$Pbam$ (55)	P_aca2_1 (29.104)	$mm21'$	G-wP	×
1.55	Na_2MnF_5	$P2_1/c$ (14)	P_bc (7.29)	$m1'$	G-wP	×
1.56	$Gd_2Ti_2O_7$	$Fd\bar{3}m$ (227)	$R_I\bar{3}m$ (166.102)	$\bar{3}m1'$	×	×
1.57	$CuMnO_2$	$C2/m$ (12)	$P_S\bar{1}$ (2.7)	$\bar{1}1'$	×	×
1.58	$La_2O_2Fe_2OSe_2$	$I4/mmm$ (139)	C_cc (9.40)	$m1'$	G-wP	×
1.59	KTb_3F_{12}	$I4/m$ (87)	P_I42/m (84.58)	$4/m1'$	×	×
1.60	$Ca_3Co_2O_6$	$R\bar{3}c$ (167)	P_C2_1/c (14.84)	$2/m1'$	×	×
1.61	$MnWO_4$	$P2/c$ (13)	C_a2/c (15.91)	$2/m1'$	×	×
1.62	CuO	$C2/c$ (15)	P_a2_1/c (14.80)	$2/m1'$	×	×
1.63	$MnPb_4Sb_6S_{14}$	$P2_1/c$ (14)	P_a2_1/c (14.80)	$2/m1'$	×	×
1.64	$BaNiF_4$	$Cmc2_1$ (36)	P_a2_1 (4.10)	$21'$	G-woP	×
1.65	$SrFeO_2$	$P4/mmm$ (123)	F_Smmm (69.526)	$mmm1'$	×	×
1.66	$Fe(ND_3)_2PO_4$	$P2_1/n$ (14)	$P_S\bar{1}$ (2.7)	$\bar{1}1'$	×	×
1.67	TmPtIn	$P\bar{6}2m$ (189)	A_bbm2 (39.201)	$mm21'$	G-woP	×
1.68	$NaNdFeWO_6$	$P2_1$ (4)	P_S1 (1.3)	$11'$	G-woP	×
1.69	CoO	$Fm\bar{3}m$ (225)	C_c2/c (15.90)	$2/m1'$	×	×
1.70	CoV_2O_6	$C2/m$ (12)	C_c2/c (15.90)	$2/m1'$	×	×
1.71	$SrCo_2V_2O_8$	$I4_1cd$ (110)	P_Ica2_1 (29.110)	$mm21'$	G-woP	×
1.72	Sr_2CoOsO_6	$I4/m$ (87)	C_c2/c (15.90)	$2/m1'$	×	×
1.73	CaV_2O_4	$P2_1/n11$ (14)	P_a2_1/c (14.80)	$2/m1'$	×	×
1.74	$BiMn_2O_5$	$Pbam$ (55)	C_amc2_1 (36.178)	$mm21'$	G-wP	×
1.75	$BiMn_2O_5$	$Pbam$ (55)	C_am (8.36)	$m1'$	G-wP	×

Continued on next page

Suppl. Tab. XI – continued from previous page

BCS-ID	Formula	**Parent**	**MSG**	**MPG**	**SHG type**	**LMO**
1.76	$DyMn_2O_5$	$Pbam$ (55)	P_aca2_1 (29.104)	$mm21'$	G-wP	×
1.77	Sr_2IrO_4	$I4_1/acd$ (142)	P_Icca (54.352)	$mmm1'$	×	×
1.78	Li_2MnSiO_4	$P2_1/n$ (14)	P_a2_1/c (14.80)	$2/m1'$	×	×
1.79	Li_2CoSiO_4	$Pna2_1$ (33)	C_ac (9.41)	$m1'$	G-woP	×
1.80	Dy_2CoGa_8	$P4/mmm$ (123)	I_c4/mcm (140.550)	$4/mmm1'$	×	×
1.81	$GdIn_3$	$Pm\bar{3}m$ (221)	P_C4/mbm (127.397)	$4/mmm1'$	×	×
1.82	Nd_2RhIn_8	$P4/mmm$ (123)	I_c4/mcm (140.550)	$4/mmm1'$	×	×
1.83	$BaFeO_{2.5}$	$P2_1/c$ (14)	P_a2_1/c (14.80)	$2/m1'$	×	×
1.84	$SrFeO_2F$	$Pm\bar{3}m$ (221)	I_c4/mcm (140.550)	$4/mmm1'$	×	×
1.85	alpha-Mn	$I\bar{4}3m$ (217)	$P_I\bar{4}2_1c$ (114.282)	$\bar{4}2m1'$	G-woP	×
1.86	GeV_4S_8	$F\bar{4}3m$ (216)	P_ana2_1 (33.149)	$mm21'$	G-woP	×
1.87	Tb_2CoGa_8	$P4/mmm$ (123)	I_c4/mcm (140.550)	$4/mmm1'$	×	×
1.88	Mn_5Si_3	$P6_3/mcm$ (193)	P_Cbcn (60.431)	$mmm1'$	×	×
1.89	$DyFe_3(BO_3)_4$	$P312_1$ (152)	P_c322_1 (154.44)	$321'$	G-woP	×
1.90	$YFe_3(BO_3)_4$	$P312_1$ (152)	C_c2 (5.16)	$21'$	G-woP	×
1.91	$TbFe_3(BO_3)_4$	$P312_1$ (152)	P_c322_1 (154.44)	$321'$	G-woP	×
1.92	$HoFe_3(BO_3)_4$	$P312_1$ (152)	P_c322_1 (154.44)	$321'$	G-woP	×
1.93	$HoFe_3(BO_3)_4$	$P312_1$ (152)	P_S1 (1.3)	$11'$	G-woP	×
1.94	$Ba_3LaRu_2O_9$	$P6_3/mmc$ (194)	P_C2_1/c (14.84)	$2/m1'$	×	×
1.95	$BaNd_2O_4$	$Pnam$ (62)	P_a2_1/c (14.80)	$2/m1'$	×	×
1.96	$BaNd_2O_4$	$Pnam$ (62)	P_a2_1/c (14.80)	$2/m1'$	×	×
1.97	Li_2MnO_3	$C2/m$ (12)	C_c2/m (12.63)	$2/m1'$	×	×
1.98	$DyFe_4Ge_2$	$P4_2/mnm$ (136)	P_ccc2 (27.82)	$mm21'$	G-wP	×
1.99	$CsCoCl_3(D_2O)_2$	$Pcca$ (54)	P_bccn (56.372)	$mmm1'$	×	×
1.100	Cu_2MnSnS_4	$I\bar{4}2m$ (121)	C_c2 (5.16)	$21'$	G-woP	×
1.101	$LuMnO_3$	$Pbnm$ (62)	P_bmn2_1 (31.129)	$mm21'$	G-wP	×
1.102	U_2Ni_2In	$P4/mbm$ (127)	P_c4/mnc (128.408)	$4/mmm1'$	×	×
1.103	U_2Rh_2Sn	$P4/mbm$ (127)	P_c4_2/mbc (135.492)	$4/mmm1'$	×	×
1.104	Gd_2CuO_4	$I4/mmm$ (139)	C_Accm (66.5)	$mmm1'$	×	×
1.105	Gd_2CuO_4	$Aeam$ (64)	P_Accn (56.374)	$mmm1'$	×	×
1.106	Pr_2CuO_4	$I4/mmm$ (139)	C_Accm (66.5)	$mmm1'$	×	×
1.107	Sm_2CuO_4	$I4/mmm$ (139)	C_Amca (64.480)	$mmm1'$	×	×
1.108	$TbMn_2O_5$	$Pbam$ (55)	C_am (8.36)	$m1'$	G-wP	×
1.109	$HoMn_2O_5$	$Pbam$ (55)	C_am (8.36)	$m1'$	G-wP	×
1.110	$ScMn_6Ge_6$	$P6/mmm$ (191)	P_c6/mcc (192.252)	$6/mmm1'$	×	×
1.111	GdBiPt	$F\bar{4}3m$ (216)	C_cc (9.40)	$m1'$	G-woP	×
1.112	$NiTa_2O_6$	$P4_2/mnm$ (136)	P_c2_1/c (14.82)	$2/m1'$	×	×
1.113	$NiSb_2O_6$	$P4_2/mnm$ (136)	$P_S\bar{1}$ (2.7)	$\bar{1}1'$	×	×
1.114	Ca_4IrO_6	$R\bar{3}c$ (167)	P_C2/c (13.74)	$2/m1'$	×	×
1.115	$Dy_3Ru_4Al_{12}$	$P6_3/mmc$ (194)	C_c2/c (15.90)	$2/m1'$	×	×
1.116	$AgMnVO_4$	$Pnma$ (62)	P_a2_1/m (11.55)	$2/m1'$	×	×
1.117	$NaFePO_4$	$Pnma$ (62)	P_c2_1/c (14.82)	$2/m1'$	×	×
1.118	$GdPO_4$	$P2_1/n$ (14)	P_a2_1/c (14.80)	$2/m1'$	×	×
1.119	$LaMn_3V_4O_{12}$	$Im\bar{3}$ (204)	$R_I\bar{3}$ (148.20)	$\bar{3}1'$	×	×
1.120	$BaFe_2Se_3$	$Pnma$ (62)	C_ac (9.41)	$m1'$	G-wP	×
1.121	$NaFeSO_4F$	$C2/c$ (15)	P_C2/c (13.74)	$2/m1'$	×	×
1.122	$Cu_3Bi(SeO_3)_2O_2Br$	$Pmmn$ (59)	P_cccn (56.373)	$mmm1'$	×	×
1.123	$Cu_3Y(SeO_3)_2O_2Cl$	$Pmmn$ (59)	P_cccn (56.373)	$mmm1'$	×	×
1.124	$YBaFe_4O_7$	$P2_1$ (4)	P_a2_1 (4.10)	$21'$	G-woP	×
1.125	LaFeAsO	$Cmme$ (67)	I_cbca (73.553)	$mmm1'$	×	×
1.126	$NaCoSO_4F$	$C2/c$ (15)	P_C2/c (13.74)	$2/m1'$	×	×

Continued on next page

Suppl. Tab. XI – continued from previous page

BCS-ID	Formula	Parent	MSG	MPG	SHG type	LMO
1.127	$BiNiO(PO_4)$	$P2_1/n$ (14)	P_a2_1/c (14.80)	$2/m1'$	×	×
1.128	$BiCoO(PO_4)$	$P2_1/n$ (14)	P_a2_1/c (14.80)	$2/m1'$	×	×
1.129	$AgFe_3(SO_4)_2(OD)_6$	$R\bar{3}m$ (166)	$R_I\bar{3}c$ (167.108)	$\bar{3}m1'$	×	×
1.130	Cr_2As	$P4/nmm$ (129)	P_anma (62.450)	$mmm1'$	×	×
1.131	Fe_2As	$P4/nmm$ (129)	P_anma (62.450)	$mmm1'$	×	×
1.132	Mn_2As	$P4/nmm$ (129)	P_anma (62.450)	$mmm1'$	×	×
1.133	$CuSb_2O_6$	$P2_1/n$ (14)	P_a2_1/c (14.80)	$2/m1'$	×	×
1.134	$Co_2C10O_8H_2$	$C2/m$ (12)	P_C2_1/m (11.57)	$2/m1'$	×	×
1.135	$C_8H10Co_2O_{11}$	$P\bar{1}$ (2)	$P_S\bar{1}$ (2.7)	$\bar{1}1'$	×	×
1.136	$AgCrS_2$	$R3m$ (160)	C_cm (8.35)	$m1'$	G-woP	×
1.137	Sr_2CaIrO_6	$P2_1/n$ (14)	$P_S\bar{1}$ (2.7)	$\bar{1}1'$	×	×
1.138	MgV_2O_4	$I\bar{4}m2$ (119)	C_A222_1 (20.37)	$2221'$	G-woP	×
1.139	Ho_2RhIn_8	$P4/mmm$ (123)	P_cccm (49.273)	$mmm1'$	×	×
1.140	PrMgPb	$I4/mmm$ (139)	P_A2/c (13.73)	$2/m1'$	×	×
1.141	NdMgPb	$I4/mmm$ (139)	P_A2/c (13.73)	$2/m1'$	×	×
1.142	CeMgPb	$I4/mmm$ (139)	C_Amma (67.510)	$mmm1'$	×	×
1.143	Mn_3Pt	$Pm\bar{3}m$ (221)	P_c4_2/mcm (132.456)	$4/mmm1'$	×	×
1.144	$NH_4FeCl_2(HCOO)$	$C2/c$ (15)	P_C2_1/c (14.84)	$2/m1'$	×	×
1.145	$Mn_3Ni_20P_6$	$Fm\bar{3}m$ (225)	C_Amca (64.480)	$mmm1'$	×	×
1.146	LaCrAsO	$P4/nmm$ (129)	P_c4_2/ncm (138.528)	$4/mmm1'$	×	×
1.147	$Li_2Fe(SO_4)_2$	$P2_1/c$ (14)	P_a2_1/c (14.80)	$2/m1'$	×	×
1.148	$CeOs_{1.84}Ir_{0.16}Al_10$	$Cmcm$ (63)	P_Anma (62.453)	$mmm1'$	×	×
1.149	$La_{0.8}Bi_{0.2}Mn_2O_5$	$Pbam$ (55)	P_cbam (55.361)	$mmm1'$	×	×
1.150	PrAg	$Pm\bar{3}m$ (221)	P_Bmna (53.334)	$mmm1'$	×	×
1.151	$Mn_{0.375}Co_{0.375}Fe_{0.25}$	$Fm\bar{3}m$ (225)	P_A2_1/c (14.83)	$2/m1'$	×	×
1.152	Ce_3NIn	$Pm\bar{3}m$ (221)	$P_C\bar{4}b2$ (117.305)	$\bar{4}2m1'$	G-wP	×
1.153	Mn_3GaC	$Pm\bar{3}m$ (221)	$R_I\bar{3}c$ (167.108)	$\bar{3}m1'$	×	×
1.154	$NaFeSi_2O_6$	$C2/c$ (15)	P_C2_1/c (14.84)	$2/m1'$	×	×
1.155	$LiFeSO_4F$	$P\bar{1}$ (2)	$P_S\bar{1}$ (2.7)	$\bar{1}1'$	×	×
1.156	$LaMn_3Cr_4O_{12}$	$Im\bar{3}$ (204)	R_I3 (146.12)	$31'$	G-wP	×
1.157	$FeF_3(H_2O)_2H_2O$	$P4/n$ (85)	P_b2_1/c (14.81)	$2/m1'$	×	×
1.158	$YMn_3Al_4O_{12}$	$Im\bar{3}$ (204)	P_Innm (58.404)	$mmm1'$	×	×
1.159	$Li_2Ni(WO_4)_2$	$P\bar{1}$ (2)	$P_S\bar{1}$ (2.7)	$\bar{1}1'$	×	×
1.160	UP	$Fm\bar{3}m$ (225)	P_I4/mnc (128.410)	$4/mmm1'$	×	×
1.161	$PrFe_3(BO_3)_4$	$R32$ (155)	R_I32 (155.48)	$321'$	G-woP	×
1.162	NdMg	$Pm\bar{3}m$ (221)	P_c4/mcc (124.360)	$4/mmm1'$	×	×
1.163	TmPdIn	$P\bar{6}2m$ (189)	$P_c\bar{6}$ (174.136)	$\bar{6}1'$	G-woP	×
1.164	Co_3TeO_6	$C2/c$ (15)	$P_S\bar{1}$ (2.7)	$\bar{1}1'$	×	×
1.165	Ni_3TeO_6	$R3$ (146)	R_I3 (146.12)	$31'$	G-woP	×
1.166	La_2LiOsO_6	$P2_1/n$ (14)	$P_S\bar{1}$ (2.7)	$\bar{1}1'$	×	×
1.167	NiS_2	$Pa\bar{3}$ (205)	$P_S\bar{1}$ (2.7)	$\bar{1}1'$	×	×
1.168	Sr_2CuTeO_6	$I4/m$ (87)	C_c2/c (15.90)	$2/m1'$	×	×
1.169	$CaCoGe_2O_6$	$C2/c$ (15)	P_C2_1/c (14.84)	$2/m1'$	×	×
1.170	$Tm_5Ni_2In_4$	$Pbam$ (55)	C_am (8.36)	$m1'$	G-wP	×
1.171	$Tb_2Fe_2Si_2C$	$C2/m$ (12)	C_c2/m (12.63)	$2/m1'$	×	×
1.172	$NiTa_2O_6$	$P4_2/mnm$ (136)	A_bba2 (41.217)	$mm21'$	G-wP	×
1.173	$La_{0.375}Ca_{0.625}MnO_3$	$Pnma$ (62)	P_bmc2_1 (26.72)	$mm21'$	G-wP	×
1.174	$La_{0.333}Ca_{0.667}MnO_3$	$Pnma$ (62)	P_bmc2_1 (26.72)	$mm21'$	G-wP	×
1.175	$La_{0.333}Ca_{0.667}MnO_3$	$Pbnm$ (62)	P_bmn2_1 (31.129)	$mm21'$	G-wP	×
1.176	$YbCo_2Si_2$	$I4/mmm$ (139)	I_cbca (73.553)	$mmm1'$	×	×
1.177	Sr_2CuWO_6	$I4/m$ (87)	$P_S\bar{1}$ (2.7)	$\bar{1}1'$	×	×

Continued on next page

Suppl. Tab. XI – continued from previous page

BCS-ID	Formula	Parent	MSG	MPG	SHG type	LMO
1.178	$Cu_{1.07}Mn_{0.93}O_2$	$C2/m$ (12)	$P_S\bar{1}$ (2.7)	$\bar{1}1'$	×	×
1.179	$NdCoAsO$	$P4/nmm$ (129)	P_anma (62.450)	$mmm1'$	×	×
1.180	$Na_3Co_2SbO_6$	$C2/m$ (12)	$P_S\bar{1}$ (2.7)	$\bar{1}1'$	×	×
1.181	$Ba_3Fe_3O_7F$	$P2_1/m$ (11)	P_a2_1/m (11.55)	$2/m1'$	×	×
1.182	$TlMnO_3$	$Pm\bar{3}m$ (221)	$P_S\bar{1}$ (2.7)	$\bar{1}1'$	×	×
1.183	$FePS_3$	$C2/m$ (12)	C_c2/m (12.63)	$2/m1'$	×	×
1.184	$Na_2Co_2TeO_6$	$P6_322$ (182)	$P_C2_12_12_1$ (19.29)	$2221'$	G-woP	×
1.185	$GeCu_2O_4$	$I4_1/amd$ (141)	$I_c\bar{4}2d$ (122.338)	$\bar{4}2m1'$	G-wP	×
1.186	$SrRu_2O_6$	$P\bar{3}1m$ (162)	$P_c\bar{3}1m$ (162.78)	$\bar{3}m1'$	×	×
1.187	$TbRh_2Si_2$	$I4/mmm$ (139)	P_I4/mnc (128.410)	$4/mmm1'$	×	×
1.188	$CeRh_2Si_2$	$I4/mmm$ (139)	C_Amca (64.480)	$mmm1'$	×	×
1.189	$TbMg_3$	$Fm\bar{3}m$ (225)	$R_I\bar{3}c$ (167.108)	$\bar{3}m1'$	×	×
1.190	$YCr(BO_3)_2$	$R\bar{3}$ (148)	$P_S\bar{1}$ (2.7)	$\bar{1}1'$	×	×
1.191	$HoCr(BO_3)_2$	$R\bar{3}$ (148)	$P_S\bar{1}$ (2.7)	$\bar{1}1'$	×	×
1.192	$SmMn_2O_5$	$Pbam$ (55)	P_bmc2_1 (26.72)	$mm21'$	G-wP	×
1.193	$CrTe_3$	$P2_1/c$ (14)	$P_S\bar{1}$ (2.7)	$\bar{1}1'$	×	×
1.194	$NiWO_4$	$P2/c$ (13)	P_a2/c (13.70)	$2/m1'$	×	×
1.195	Er_2Ni_2In	$Cmmm$ (65)	C_amcm (63.467)	$mmm1'$	×	×
1.196	MnV_2O_6	$Pbcn$ (60)	P_a2_1/c (14.80)	$2/m1'$	×	×
1.197	$Fe_4Si_2Sn_7O_{16}$	$P\bar{3}m1$ (164)	C_c2/m (12.63)	$2/m1'$	×	×
1.198	$Ni_{1.64}Co_{0.36}Mn_{1.28}Ga_{0.72}$	$I4/mmm$ (139)	P_I4_2/mnm (136.506)	$4/mmm1'$	×	×
1.199	Sc_2NiMnO_6	$P2_1/c$ (14)	P_a2_1/c (14.80)	$2/m1'$	×	×
1.200	U_2Ni_2Sn	$P4/mbm$ (127)	C_cmcm (63.466)	$mmm1'$	×	×
1.201	Cr_2ReO_6	$P4_2/mnm$ (136)	P_a2_1/c (14.80)	$2/m1'$	×	×
1.202	$CrReO_4$	$C2/m$ (12)	C_c2/c (15.90)	$2/m1'$	×	×
1.203	Ni_2SiO_4	$Pnma$ (62)	P_c2_1/c (14.82)	$2/m1'$	×	×
1.204	Ni_2SiO_4	$Pnma$ (62)	P_c2_1/c (14.82)	$2/m1'$	×	×
1.205	$Dy_2Fe_2Si_2C$	$C2/m$ (12)	C_c2/m (12.63)	$2/m1'$	×	×
1.206	$Dy_2Fe_2Si_2C$	$C2/m$ (12)	$P_S\bar{1}$ (2.7)	$\bar{1}1'$	×	×
1.207	U_2Rh_2Sn	$P4/mbm$ (127)	P_c4_2/mbc (135.492)	$4/mmm1'$	×	×
1.208	UAs	$Fm\bar{3}m$ (225)	P_I4/mnc (128.410)	$4/mmm1'$	×	×
1.209	FeI_2	$P\bar{3}m1$ (164)	C_c2/c (15.90)	$2/m1'$	×	×
1.210	$FePSe_3$	$R\bar{3}$ (148)	$P_S\bar{1}$ (2.7)	$\bar{1}1'$	×	×
1.211	Dy_2O_2S	$P\bar{3}m1$ (164)	C_c2/c (15.90)	$2/m1'$	×	×
1.212	Dy_2O_2Se	$P\bar{3}m1$ (164)	C_c2/c (15.90)	$2/m1'$	×	×
1.213	Ho_2O_2Se	$P\bar{3}m1$ (164)	P_A2/c (13.73)	$2/m1'$	×	×
1.214	Yb_2O_2Se	$P\bar{3}m1$ (164)	C_c2/c (15.90)	$2/m1'$	×	×
1.215	UP_2	$P4/nmm$ (129)	P_c4/ncc (130.432)	$4/mmm1'$	×	×
1.216	Nd_2BaNiO_5	$Immm$ (71)	C_c2/c (15.90)	$2/m1'$	×	×
1.217	Tb_2BaNiO_5	$Immm$ (71)	C_c2/c (15.90)	$2/m1'$	×	×
1.218	Tm_2BaNiO_5	$Immm$ (71)	$P_S\bar{1}$ (2.7)	$\bar{1}1'$	×	×
1.219	CuF_2	$P2_1/c$ (14)	$P_S\bar{1}$ (2.7)	$\bar{1}1'$	×	×
1.220	$YBa_2Fe_3O_{8.08}$	$P4/mmm$ (123)	I_bmma (74.562)	$mmm1'$	×	×
1.221	$YBa_2Fe_3O_{7.84}$	$Pmmm$ (47)	C_a2/m (12.64)	$2/m1'$	×	×
1.222	Er_2CoGa_8	$P4/mmm$ (123)	P_amma (51.298)	$mmm1'$	×	×
1.223	Tm_2CoGa_8	$P4/mmm$ (123)	C_ammm (65.489)	$mmm1'$	×	×
1.224	$CoNb_2O_6$	$Pbcn$ (60)	$P_c2_12_12_1$ (19.28)	$2221'$	G-wP	×
1.225	$ScMn_6Ge_6$	$P6/mmm$ (191)	P_c6/mcc (192.252)	$6/mmm1'$	×	×
1.226	$CeCo_2Ge_4O_{12}$	$P4/nbm$ (125)	P_bnna (52.315)	$mmm1'$	×	×
1.227	$Ca_2Cr_2O_5$	$I2mb$ (46)	P_C2_1 (4.12)	$21'$	G-woP	×
1.228	$RuCl_3$	$C2/m$ (12)	P_C2/m (10.49)	$2/m1'$	×	×

Continued on next page

Suppl. Tab. XI – continued from previous page

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

Continued on next page

Suppl. Tab. XI – continued from previous page

BCS-ID	Formula	Parent	MSG	MPG	SHG type	LMO
1.280	$Yb_2Cu_2O_5$	$Pna2_1$ (33)	P_ac (7.27)	$m1'$	G-woP	×
1.281	$YBaCuFeO_5$	$P4mm$ (99)	F_Smm2 (42.223)	$mm21'$	G-woP	×
1.282	$YBaCuFeO_5$	$P4/mmm$ (123)	C_a2/m (12.64)	$2/m1'$	×	×
1.283	$YBaCuFeO_5$	$P4/mmm$ (123)	C_a2/m (12.64)	$2/m1'$	×	×
1.284	$YBaCuFeO_5$	$P4/mmm$ (123)	C_a2/m (12.64)	$2/m1'$	×	×
1.285	$YBaCuFeO_5$	$P4/mmm$ (123)	F_Smmm (69.526)	$mmm1'$	×	×
1.286	$Fe_2(C_2O_4)_{3.4}H_2O$	$P\bar{1}$ (2)	$P_S\bar{1}$ (2.7)	$\bar{1}1'$	×	×
1.287	V_2O_3	$I2/a$ (15)	P_C2_1/c (14.84)	$2/m1'$	×	×
1.288	$CePd_2Si_2$	$I4/mmm$ (139)	C_Accm (66.5)	$mmm1'$	×	×
1.289	$CePd_2Ge_2$	$I4/mmm$ (139)	C_Accm (66.5)	$mmm1'$	×	×
1.290	$CeRh_2Si_2$	$I4/mmm$ (139)	C_Amca (64.480)	$mmm1'$	×	×
1.291	$CeAu_2Si_2$	$I4/mmm$ (139)	P_I4/mnc (128.410)	$4/mmm1'$	×	×
1.292	$HoNi_2B_2C$	$I4/mmm$ (139)	C_Amca (64.480)	$mmm1'$	×	×
1.293	$NdNi_2B_2C$	$I4/mmm$ (139)	C_c2/c (15.90)	$2/m1'$	×	×
1.294	$HoNi_2B_2C$	$I4/mmm$ (139)	C_Amca (64.480)	$mmm1'$	×	×
1.295	$DyNi_2B_2C$	$I4/mmm$ (139)	C_Amca (64.480)	$mmm1'$	×	×
1.296	$PrNi_2B_2C$	$I4/mmm$ (139)	C_Amca (64.480)	$mmm1'$	×	×
1.297	$CuFe_2(P_2O_7)_2$	$P2_1/n$ (14)	P_a2_1/c (14.80)	$2/m1'$	×	×
1.298	$BaCdVO(PO_4)_2$	$Pbca$ (61)	P_bna2_1 (33.150)	$mm21'$	G-wP	×
1.299	$GdMn_2O_5$	$Pbam$ (55)	P_aca2_1 (29.104)	$mm21'$	G-wP	×
1.300	$GdMn_2O_5$	$Pbam$ (55)	P_aca2_1 (29.104)	$mm21'$	G-wP	×
1.301	$BiMnTeO_6$	$P2_1/c$ (14)	P_a2_1/c (14.80)	$2/m1'$	×	×
1.302	Ba_2CoO_4	$P2_1/n$ (14)	P_a2_1/c (14.80)	$2/m1'$	×	×
1.303	$Dy_3Ru_4Al_{12}$	$P6_3/mmc$ (194)	C_c2/c (15.90)	$2/m1'$	×	×
1.304	$ZnMnO_3$	$R\bar{3}$ (148)	$P_S\bar{1}$ (2.7)	$\bar{1}1'$	×	×
1.305	Mn_5Si_3	$P6_3/mcm$ (193)	P_Cbcn (60.431)	$mmm1'$	×	×
1.306	$Na_2BaMn(VO_4)_2$	$C2/c$ (15)	P_C2_1/c (14.84)	$2/m1'$	×	×
1.307	Mn_5Si_3	$P6_3/mcm$ (193)	P_S1 (1.3)	$11'$	G-wP	×
1.308	$MnBi_2Te_4$	$R\bar{3}m$ (166)	$R_I\bar{3}c$ (167.108)	$\bar{3}m1'$	×	×
1.309	$MnBi_2Te_4$	$R\bar{3}m$ (166)	$R_I\bar{3}c$ (167.108)	$\bar{3}m1'$	×	×
1.310	$MnBi_4Te_7$	$P\bar{3}m1$ (164)	$P_c\bar{3}c1$ (165.96)	$\bar{3}m1'$	×	×
1.311	$BaMo(PO_4)_2$	$C2/m$ (12)	$P_S\bar{1}$ (2.7)	$\bar{1}1'$	×	×
1.312	$HoNi_2B_2C$	$I4/mmm$ (139)	C_Amca (64.480)	$mmm1'$	×	×
1.313	$GdFeZnGe_4O_{12}$	$P4/nbm$ (125)	P_bnna (52.315)	$mmm1'$	×	×
1.314	$NaFeSi_2O_6$	$C2/c$ (15)	P_C2_1/c (14.84)	$2/m1'$	×	×
1.315	$Mn_{0.8}1Cu_{0.19}WO_4$	$P2/c$ (13)	P_a2/c (13.70)	$2/m1'$	×	×
1.316	$La_{0.25}Pr_{0.75}Co_2P_2$	$I4/mmm$ (139)	P_c4/mcc (124.360)	$4/mmm1'$	×	×
1.317	$La_{0.25}Pr_{0.75}Co_2P_2$	$I4/mmm$ (139)	C_c2/c (15.90)	$2/m1'$	×	×
1.318	$Sr_2Ru_{0.95}Fe_{0.05}O_4$	$I4/mmm$ (139)	C_cmca (64.478)	$mmm1'$	×	×
1.319	$Sr_2Ru_{0.95}Fe_{0.05}O_4$	$I4/mmm$ (139)	C_cmcm (63.466)	$mmm1'$	×	×
1.320	Sr_2FeWO_6	$P2_1/n$ (14)	$P_S\bar{1}$ (2.7)	$\bar{1}1'$	×	×
1.321	Ba_2FeWO_6	$I4/m$ (87)	$P_S\bar{1}$ (2.7)	$\bar{1}1'$	×	×
1.322	Sr_2FeWO_5N	$I4/m$ (87)	$P_S\bar{1}$ (2.7)	$\bar{1}1'$	×	×
1.323	$CoGeO_3$	$C2/c$ (15)	P_C2_1/c (14.84)	$2/m1'$	×	×
1.324	$DyMn_2O_5$	$Pbam$ (55)	P_aca2_1 (29.104)	$mm21'$	G-wP	×
1.325	$PrMn_2O_5$	$Pbam$ (55)	P_cc (7.28)	$m1'$	G-wP	×
1.326	$PrMn_2O_5$	$Pbam$ (55)	P_bnma (62.451)	$mmm1'$	×	×
1.327	$LaMn_2O_5$	$Pbam$ (55)	P_cbam (55.361)	$mmm1'$	×	×
1.328	Yb_2CoMnO_6	$P2_1/c$ (14)	P_a2_1 (4.10)	$21'$	G-wP	×
1.329	$YbLuCoMnO_6$	$P2_1/c$ (14)	P_a2_1 (4.10)	$21'$	G-wP	×
1.330	Lu_2CoMnO_6	$P2_1/c$ (14)	P_a2_1 (4.10)	$21'$	G-wP	×

Continued on next page

Suppl. Tab. XI – continued from previous page

BCS-ID	Formula	Parent	MSG	MPG	SHG type	LMO
1.331	$Li_{0.3}1Na_{0.69}FeGe_2O_6$	$P2_1/c$ (14)	P_a2_1/c (14.80)	$2/m1'$	×	×
1.332	$Li_{0.22}Na_{0.78}FeGe_2O_6$	$C2/c$ (15)	P_C2_1/c (14.84)	$2/m1'$	×	×
1.333	$Yb_2Pd_2(In_{0.4}Sn_{0.6})$	$P4/mbm$ (127)	P_c4/mbm (127.396)	$4/mmm1'$	×	×
1.334	Pr_2Pd_2In	$P4/mbm$ (127)	P_bnma (62.451)	$mmm1'$	×	×
1.335	Nd_2Pd_2In	$P4/mbm$ (127)	P_cmc2_1 (26.73)	$mm21'$	G-wP	×
1.336	$Tb_2Pd_2.0_5Sn_{0.95}$	$P4/mbm$ (127)	P_bnma (62.451)	$mmm1'$	×	×
1.337	$U_2Pd_{2.35}Sn_{0.65}$	$P4/mbm$ (127)	P_c4/mnc (128.408)	$4/mmm1'$	×	×
1.338	U_2Ni_2In	$P4/mbm$ (127)	P_c4/mnc (128.408)	$4/mmm1'$	×	×
1.339	$EuAs_3$	$C2/m$ (12)	C_c2/m (12.63)	$2/m1'$	×	×
1.340	$LuMnO_3$	$Pbnm$ (62)	P_bmn2_1 (31.129)	$mm21'$	G-wP	×
1.341	$TmMnO_3$	$Pnma$ (62)	P_bmn2_1 (31.129)	$mm21'$	G-wP	×
1.342	$Co_3(PO_4)_2$	$P2_1/c$ (14)	P_a2_1/c (14.80)	$2/m1'$	×	×
1.343	$Ba_2Co_9O_{14}$	$R\bar{3}m$ (166)	C_c2/c (15.90)	$2/m1'$	×	×
1.344	$Ba_2Co_9O_{14}$	$R\bar{3}m$ (166)	C_c2/m (12.63)	$2/m1'$	×	×
1.345	$NaMnF_4$	$P2_1/c$ (14)	P_a2_1/c (14.80)	$2/m1'$	×	×
1.346	$TlMnF_4$	$I2/a$ (15)	P_C2/c (13.74)	$2/m1'$	×	×
1.347	$CuFeO_2$	$R\bar{3}m$ (166)	C_a2/c (15.91)	$2/m1'$	×	×
1.348	$CuFeO_2$	$R\bar{3}m$ (166)	C_c2/c (15.90)	$2/m1'$	×	×
1.349	$CoNb_3S_6$	$P6_322$ (182)	$P_B2_12_12$ (18.22)	$2221'$	G-woP	×
1.350	Nd_2BaCoO_5	$Immm$ (71)	C_c2/c (15.90)	$2/m1'$	×	×
1.351	$Ba_2Co_2F_7Cl$	$P2_1/m$ (11)	P_a2_1/m (11.55)	$2/m1'$	×	×
1.352	$Ba_2Ni_2F_7Cl$	$P2_1/m$ (11)	P_c2_1/c (14.82)	$2/m1'$	×	×
1.353	$SmNiO_3$	$Pnma$ (62)	C_amc2_1 (36.178)	$mm21'$	G-wP	×
1.354	$EuNiO_3$	$Pnma$ (62)	C_amc2_1 (36.178)	$mm21'$	G-wP	×
1.355	$DyGe_3$	$Cmcm$ (63)	P_a2_1/m (11.55)	$2/m1'$	×	×
1.356	Ho_3Ge_4	$Cmcm$ (63)	P_Bnna (52.318)	$mmm1'$	×	×
1.357	Ho_3Ge_4	$Cmcm$ (63)	P_c2_1/c (14.82)	$2/m1'$	×	×
1.358	$HoGe_{1.5}$	$P6/mmm$ (191)	C_cmcm (63.466)	$mmm1'$	×	×
1.359	Dy_3Ge_4	$Cmcm$ (63)	P_a2_1/m (11.55)	$2/m1'$	×	×
1.360	$DyGe_{1.3}$	$P6/mmm$ (191)	C_cmcm (63.466)	$mmm1'$	×	×
1.361	DyGe	$Cmcm$ (63)	C_c2/c (15.90)	$2/m1'$	×	×
1.362	Er_3Ge_4	$Cmcm$ (63)	P_Cbcm (57.391)	$mmm1'$	×	×
1.363	$TbCu_2Si_2$	$I4/mmm$ (139)	$P_S\bar{1}$ (2.7)	$\bar{1}1'$	×	×
1.364	$HoCu_2Si_2$	$I4/mmm$ (139)	$P_S\bar{1}$ (2.7)	$\bar{1}1'$	×	×
1.365	$TbCu_2Si_2$	$I4/mmm$ (139)	$P_S\bar{1}$ (2.7)	$\bar{1}1'$	×	×
1.366	$HoCu_2Si_2$	$I4/mmm$ (139)	C_c2/m (12.63)	$2/m1'$	×	×
1.367	Pu_2O_3	$P\bar{3}m1$ (164)	C_c2/c (15.90)	$2/m1'$	×	×
1.368	$Tb_2Ni_3Si_5$	$Ibam$ (72)	P_Ibam (55.364)	$mmm1'$	×	×
1.369	HFe_2Ge_2	$I4/mmm$ (139)	C_Amca (64.480)	$mmm1'$	×	×
1.370	Li_2CuO_2	$Immm$ (71)	P_Innm (58.404)	$mmm1'$	×	×
1.371	Nd_2NiO_4	$Cmce$ (64)	P_Cmna (53.335)	$mmm1'$	×	×
1.372	$Sr_2MnO_2Ag_{1.5}Se_2$	$I4/mmm$ (139)	P_I4/mnc (128.410)	$4/mmm1'$	×	×
1.373	$Li_3Ni_2SbO_6$	$C2/m$ (12)	$P_S\bar{1}$ (2.7)	$\bar{1}1'$	×	×
1.374	HoNiGe	$Pnma$ (62)	P_cc (7.28)	$m1'$	G-wP	×
1.375	CeScGe	$I4/mmm$ (139)	$P_S\bar{1}$ (2.7)	$\bar{1}1'$	×	×
1.376	CeScGe	$I4/mmm$ (139)	C_Amcm (63.468)	$mmm1'$	×	×
1.377	CeScSi	$I4/mmm$ (139)	$P_S\bar{1}$ (2.7)	$\bar{1}1'$	×	×
1.378	CeScSi	$I4/mmm$ (139)	C_Amcm (63.468)	$mmm1'$	×	×
1.379	ErNiGe	$Pnma$ (62)	P_a2_1/c (14.80)	$2/m1'$	×	×
1.380	Sr_2FeO_3Cl	$P4/nmm$ (129)	$P_C\bar{4}2_1m$ (113.273)	$\bar{4}2m1'$	G-wP	×
1.381	Sr_2FeO_3Br	$P4/nmm$ (129)	$P_C\bar{4}2_1m$ (113.273)	$\bar{4}2m1'$	G-wP	×

Continued on next page

Suppl. Tab. XI – continued from previous page

BCS-ID	Formula	Parent	MSG	MPG	SHG type	LMO
1.382	Ca_2FeO_3Cl	$P4/nmm$ (129)	$P_C\bar{4}2_1m$ (113.273)	$\bar{4}2m1'$	G-wP	×
1.383	Ca_2FeO_3Br	$P4/nmm$ (129)	$P_C\bar{4}2_1m$ (113.273)	$\bar{4}2m1'$	G-wP	×
1.384	USb_2	$P4/nmm$ (129)	P_c4/ncc (130.432)	$4/mmm1'$	×	×
1.385	Sr_2FeO_3F	$P4/nmm$ (129)	$P_C\bar{4}2_1m$ (113.273)	$\bar{4}2m1'$	G-wP	×
1.386	Sr_2FeO_3F	$P4/nmm$ (129)	$I_c\bar{4}2m$ (121.332)	$\bar{4}2m1'$	G-wP	×
1.387	Sr_2FeO_3F	$P4/nmm$ (129)	$P_C\bar{4}2m$ (111.257)	$\bar{4}2m1'$	G-wP	×
1.388	$La_2NiO_3F_2$	$Cccm$ (66)	P_Amna (53.333)	$mmm1'$	×	×
1.389	Sr_2CoO_3Cl	$P4/nmm$ (129)	P_Bccm (49.274)	$mmm1'$	×	×
1.390	$La_2NiO_3F_{1.93}$	$C2/c$ (15)	P_C2_1/c (14.84)	$2/m1'$	×	×
1.391	Fe_2MnBO_5	$Pbam$ (55)	P_bnma (62.451)	$mmm1'$	×	×
1.392	$KCuMnS_2$	$I4/mmm$ (139)	C_Ammm (65.490)	$mmm1'$	×	×
1.393	$Pb_2BaCuFeO_5Br$	$P4/mmm$ (123)	I_bmma (74.562)	$mmm1'$	×	×
1.394	$Pb_2BaCuFeO_5Cl$	$P4/mmm$ (123)	I_bmma (74.562)	$mmm1'$	×	×
1.395	$NdCeBaCuFeO_7$	$I4/mmm$ (139)	C_Accm (66.5)	$mmm1'$	×	×
1.396	$NdCeBaCu_{0.9}Co_{1.1}O_7$	$I4/mmm$ (139)	C_Amca (64.480)	$mmm1'$	×	×
1.397	$Cu_3Mg(OD)_6Br_2$	$P\bar{3}m1$ (164)	C_c2/m (12.63)	$2/m1'$	×	×
1.398	Pr_2CuO_4	$I4/mmm$ (139)	C_Accm (66.5)	$mmm1'$	×	×
1.399	Pr_2CuO_4	$I4/mmm$ (139)	C_Accm (66.5)	$mmm1'$	×	×
1.400	$TbAg_2$	$I4/mmm$ (139)	C_Amca (64.480)	$mmm1'$	×	×
1.401	Nd_5Pb_3	$P6_3/mcm$ (193)	P_Bnma (62.454)	$mmm1'$	×	×
1.402	Nd_5Pb_3	$P6_3/mcm$ (193)	P_Bnma (62.454)	$mmm1'$	×	×
1.403	La_2CoO_4	$Cmce$ (64)	P_Cmna (53.335)	$mmm1'$	×	×
1.404	$Sr_2CuO_2Cl_2$	$I4/mmm$ (139)	C_Amca (64.480)	$mmm1'$	×	×
1.405	La_2CuO_4	$Bmeb$ (64)	P_Accn (56.374)	$mmm1'$	×	×
1.406	Nd_2CuO_4	$I4/mmm$ (139)	C_Accm (66.5)	$mmm1'$	×	×
1.407	Nd_2CuO_4	$I4/mmm$ (139)	C_Amca (64.480)	$mmm1'$	×	×
1.408	Nd_2CuO_4	$I4/mmm$ (139)	C_Accm (66.5)	$mmm1'$	×	×
1.409	$NaMnO_2$	$C2/m$ (12)	$P_S\bar{1}$ (2.7)	$\bar{1}1'$	×	×
1.410	$Sr_2Fe_{1.9}Cr_{0.1}O_5$	$Icmm$ (74)	P_Imna (53.336)	$mmm1'$	×	×
1.411	$EuMn_2P_2$	$P\bar{3}m1$ (164)	C_c2/m (12.63)	$2/m1'$	×	×
1.412	$Au_{72}Al_{14}Tb_{14}$	$Im\bar{3}$ (204)	$P_In\bar{3}$ (201.21)	$m\bar{3}1'$	×	×
1.413	$Ce_3Ni_2Ge_7$	$Cmmm$ (65)	P_Cmmn (59.415)	$mmm1'$	×	×
1.414	$CeNiGe_3$	$Cmmm$ (65)	P_Cmmn (59.415)	$mmm1'$	×	×
1.415	Tb_2Pd_2In	$P4/mbm$ (127)	C_amca (64.479)	$mmm1'$	×	×
1.416	Tb_2O_2S	$P\bar{3}m1$ (164)	C_c2/c (15.90)	$2/m1'$	×	×
1.417	Tb_2O_2Se	$P\bar{3}m1$ (164)	C_c2/c (15.90)	$2/m1'$	×	×
1.418	Cu_4O_3	$I4_1/amd$ (141)	$I_c\bar{4}2m$ (121.332)	$\bar{4}2m1'$	G-wP	×
1.419	$GdIn_3$	$Pm\bar{3}m$ (221)	P_C4/mbm (127.397)	$4/mmm1'$	×	×
1.420	$YBa_2Cu_3O_6$	$P4/mmm$ (123)	C_ammm (65.489)	$mmm1'$	×	×
1.421	$NdRh_2Si_2$	$I4/mmm$ (139)	P_I4/mnc (128.410)	$4/mmm1'$	×	×
1.422	$ErRh_2Si_2$	$I4/mmm$ (139)	P_Innm (58.404)	$mmm1'$	×	×
1.423	UPb_3	$Pm\bar{3}m$ (221)	P_c4/mcc (124.360)	$4/mmm1'$	×	×
1.424	UCu_5	$F\bar{4}3m$ (216)	R_I3c (161.72)	$3m1'$	G-woP	×
1.425	$UGeTe$	$I4/mmm$ (139)	P_I4/nnc (126.386)	$4/mmm1'$	×	×
1.426	$UGeS$	$P4/nmm$ (129)	P_c4/ncc (130.432)	$4/mmm1'$	×	×
1.427	$HoCo_2Ge_2$	$I4/mmm$ (139)	P_I4/mnc (128.410)	$4/mmm1'$	×	×
1.428	UN	$Fm\bar{3}m$ (225)	P_I4/mnc (128.410)	$4/mmm1'$	×	×
1.429	$BaFe_2Se_3$	$Pnma$ (62)	C_am (8.36)	$m1'$	G-wP	×
1.430	$Mn_5(VO_4)_2(OH)_4$	$C2/m$ (12)	P_b2/c (13.71)	$2/m1'$	×	×
1.431	$Ca_2Mn_3O_8$	$C2/m$ (12)	$P_S\bar{1}$ (2.7)	$\bar{1}1'$	×	×
1.432	Ba_2LuRuO_6	$Fm\bar{3}m$ (225)	C_Amca (64.480)	$mmm1'$	×	×

Continued on next page

Suppl. Tab. XI – continued from previous page

BCS-ID	Formula	Parent	MSG	MPG	SHG type	LMO
1.433	Ba_2YRuO_6	$Fm\bar{3}m$ (225)	C_Amca (64.480)	$mmm1'$	×	×
1.434	$Fe_{1.05}Te$	$P4/nmm$ (129)	P_a2_1/m (11.55)	$2/m1'$	×	×
1.435	$Fe_{1.05}Te$	$P4/nmm$ (129)	P_a2_1/m (11.55)	$2/m1'$	×	×
1.436	$Fe_{1.125}Te$	$P4/nmm$ (129)	$P_S\bar{1}$ (2.7)	$\bar{1}1'$	×	×
1.437	$Fe_{1.068}Te$	$P4/nmm$ (129)	$P_S\bar{1}$ (2.7)	$\bar{1}1'$	×	×
1.438	$BaCoF_4$	$A2_1am$ (36)	P_a2_1 (4.10)	$21'$	G-woP	×
1.439	$BaCoF_4$	$A2_1am$ (36)	P_bca2_1 (29.105)	$mm21'$	G-woP	×
1.440	$CrPS_4$	$C2$ (5)	C_c2 (5.16)	$21'$	G-woP	×
1.441	$NaFe_3(SO_4)_2(OH)_6$	$R\bar{3}m$ (166)	$R_I\bar{3}c$ (167.108)	$\bar{3}m1'$	×	×
1.442	URu_2Si_2	$I4/mmm$ (139)	P_I4/mnc (128.410)	$4/mmm1'$	×	×
1.443	Gd_2BaCuO_5	$Pnma$ (62)	P_aca2_1 (29.104)	$mm21'$	G-wP	×
1.444	Er_2Pt	$Pnma$ (62)	P_ana2_1 (33.149)	$mm21'$	G-wP	×
1.445	Y_2BaCuO_5	$Pnma$ (62)	P_a2_1/c (14.80)	$2/m1'$	×	×
1.446	$CeCoAl_4$	$Pmma$ (51)	C_amca (64.479)	$mmm1'$	×	×
1.447	$Ce_3Ni_2Sn_7$	$Cmmm$ (65)	P_Cmmn (59.415)	$mmm1'$	×	×
1.448	$HoSi$	$Cmcm$ (63)	C_a2/c (15.91)	$2/m1'$	×	×
1.449	$Li_2CuW_2O_8$	$P\bar{1}$ (2)	$P_S\bar{1}$ (2.7)	$\bar{1}1'$	×	×
1.450	$Pr_6Fe_{13}Sn$	$I4/mcm$ (140)	P_Ibcn (60.432)	$mmm1'$	×	×
1.451	$Nd_6Fe_{13}Sn$	$I4/mcm$ (140)	P_I4/mcc (124.362)	$4/mmm1'$	×	×
1.452	$FeSn$	$P6/mmm$ (191)	C_cmcm (63.466)	$mmm1'$	×	×
1.453	$EuMn_2Si_2$	$I4/mmm$ (139)	P_I4/nnc (126.386)	$4/mmm1'$	×	×
1.454	$Mn_6Ni_{16}Si_7$	$Fm\bar{3}m$ (225)	C_Amca (64.480)	$mmm1'$	×	×
1.455	$Mn_6Ni_{16}Si_7$	$Fm\bar{3}m$ (225)	P_A2_1/c (14.83)	$2/m1'$	×	×
1.456	$Sr_2CuO_2Cu_2S_2$	$I4/mmm$ (139)	$I_c\bar{4}2d$ (122.338)	$\bar{4}2m1'$	G-wP	×
1.457	$NdNiMg_{15}$	$P4/nmm$ (129)	P_Bcca (54.350)	$mmm1'$	×	×
1.458	$CsCo_2Se_2$	$I4/mmm$ (139)	C_Amcm (63.468)	$mmm1'$	×	×
1.459	$CeFe_3(BO_3)_4$	$R32$ (155)	C_c2 (5.16)	$21'$	G-woP	×
1.460	$PrCuSi$	$P6_3/mmc$ (194)	P_Cbcn (60.431)	$mmm1'$	×	×
1.461	$Sr_2Cr_3As_2O_2$	$I4/mmm$ (139)	P_I4_2/mnm (136.506)	$4/mmm1'$	×	×
1.462	La_2CoPtO_6	$P2_1/n$ (14)	P_a2_1/c (14.80)	$2/m1'$	×	×
1.463	$Sr_2Fe_3Se_2O_3$	$Pbam$ (55)	C_amc2_1 (36.178)	$mm21'$	G-wP	×
1.464	U_2N_2P	$P\bar{3}m1$ (164)	$P_c\bar{3}c1$ (165.96)	$\bar{3}m1'$	×	×
1.465	U_2N_2As	$P\bar{3}m1$ (164)	$P_c\bar{3}c1$ (165.96)	$\bar{3}m1'$	×	×
1.466	$MnPt_{0.5}Pd_{0.5}$	$P4/mmm$ (123)	C_amma (67.509)	$mmm1'$	×	×
1.467	$Tb_{0.6}Y_{0.4}RhIn_5$	$P4/mmm$ (123)	C_amma (67.509)	$mmm1'$	×	×
1.468	$TbMn_2Si_2$	$I4/mmm$ (139)	P_I4/nnc (126.386)	$4/mmm1'$	×	×
1.469	YMn_2Si_2	$I4/mmm$ (139)	P_I4/nnc (126.386)	$4/mmm1'$	×	×
1.470	UCr_2Si_2	$C2/m$ (12)	C_c2/c (15.90)	$2/m1'$	×	×
1.471	$EuCd_2As_2$	$P\bar{3}m1$ (164)	C_c2/m (12.63)	$2/m1'$	×	×
1.472	$CaOFeS$	$P6_3mc$ (186)	P_Cca2_1 (29.109)	$mm21'$	G-woP	×
1.473	$CuBr(C_4H_4N_2)_2(BF_4)$	$P4/nbm$ (125)	P_bnna (52.315)	$mmm1'$	×	×
1.474	$CuCl(C_4H_4N_2)_2(BF_4)$	$P4/nbm$ (125)	P_bnna (52.315)	$mmm1'$	×	×
1.475	$DyNiAl_4$	$Cmcm$ (63)	P_Anma (62.453)	$mmm1'$	×	×
1.476	Ba_2CoO_4	$P2_1/n$ (14)	P_a2_1/c (14.80)	$2/m1'$	×	×
1.477	Ba_2CoO_4	$P2_1/n$ (14)	P_a2_1/c (14.80)	$2/m1'$	×	×
1.478	$CoTi_2O_5$	$Cmcm$ (63)	P_a2_1/m (11.55)	$2/m1'$	×	×
1.479	U_2Ni_2Sn	$P4/mbm$ (127)	P_c4_2/mbc (135.492)	$4/mmm1'$	×	×
1.480	Mn_2CoReO_6	$P2_1/n$ (14)	$P_S\bar{1}$ (2.7)	$\bar{1}1'$	×	×
1.481	$LaSr_3Fe_3O_9$	$Cmcm$ (63)	P_Cbcm (57.391)	$mmm1'$	×	×
1.482	$Er_2Fe_2Si_2C$	$C2/m$ (12)	$P_S\bar{1}$ (2.7)	$\bar{1}1'$	×	×
1.483	$Eu_{0.5}Ca_{0.5}Fe_2As_2$	$Fmmm$ (69)	C_Amca (64.480)	$mmm1'$	×	×

Continued on next page

Suppl. Tab. XI – continued from previous page

BCS-ID	Formula	Parent	MSG	MPG	SHG type	LMO
1.484	Li_2MnGeO_4	$Pmn2_1$ (31)	C_ac (9.41)	$m1'$	G-woP	×
1.485	Mn_3TeO_6	$P2_1/c$ (14)	P_a2_1/c (14.80)	$2/m1'$	×	×
1.486	$CeRhAl_4Si_2$	$P4/mmm$ (123)	P_c4/mcc (124.360)	$4/mmm1'$	×	×
1.487	$CeIrAl_4Si_2$	$P4/mmm$ (123)	P_c4/mcc (124.360)	$4/mmm1'$	×	×
1.488	$CeMn_2Si_2$	$I4/mmm$ (139)	P_I4/nnc (126.386)	$4/mmm1'$	×	×
1.489	$CeMn_2Si_2$	$I4/mmm$ (139)	P_I4/nnc (126.386)	$4/mmm1'$	×	×
1.490	$CeMn_2Si_2$	$I4/mmm$ (139)	P_I4/nnc (126.386)	$4/mmm1'$	×	×
1.491	$PrMn_2Si_2$	$I4/mmm$ (139)	P_I4/nnc (126.386)	$4/mmm1'$	×	×
1.492	$PrMn_2Si_2$	$I4/mmm$ (139)	P_I4/nnc (126.386)	$4/mmm1'$	×	×
1.493	$NdMn_2Si_2$	$I4/mmm$ (139)	P_I4/nnc (126.386)	$4/mmm1'$	×	×
1.494	$NdMn_2Si_2$	$I4/mmm$ (139)	P_I4/nnc (126.386)	$4/mmm1'$	×	×
1.495	YMn_2Si_2	$I4/mmm$ (139)	P_I4/nnc (126.386)	$4/mmm1'$	×	×
1.496	YMn_2Ge_2	$I4/mmm$ (139)	P_I4/nnc (126.386)	$4/mmm1'$	×	×
1.497	$EuMg_2Bi_2$	$P\bar{3}m1$ (164)	C_c2/m (12.63)	$2/m1'$	×	×
1.498	$Cu_6(SiO_3)_6(H_2O)_6$	$R\bar{3}$ (148)	$R_I\bar{3}$ (148.20)	$\bar{3}1'$	×	×
1.499	$CsFe(MoO_4)_2$	$P\bar{3}$ (147)	P_c3 (143.3)	$31'$	G-wP	×
1.500	$Sr_2CoO_2Cu_2S_2$	$I4/mmm$ (139)	$P_S\bar{1}$ (2.7)	$\bar{1}1'$	×	×
1.501	$Ba_2CoO_2Cu_2S_2$	$I4/mmm$ (139)	$P_S\bar{1}$ (2.7)	$\bar{1}1'$	×	×
1.502	$Li_3Co_2SbO_6$	$C2/m$ (12)	C_c2/m (12.63)	$2/m1'$	×	×
1.503	$NdScSiC_{0.5}H_{0.2}$	$I4/mmm$ (139)	P_I4/nnc (126.386)	$4/mmm1'$	×	×
1.504	$GdCuSn$	$P6_3mc$ (186)	P_Cna2_1 (33.154)	$mm21'$	G-woP	×
1.505	$GdAgSn$	$P6_3mc$ (186)	P_Cna2_1 (33.154)	$mm21'$	G-woP	×
1.506	$GdAuSn$	$P6_3mc$ (186)	P_Cna2_1 (33.154)	$mm21'$	G-woP	×
1.507	$NdPd_5Al_2$	$I4/mmm$ (139)	P_anma (62.450)	$mmm1'$	×	×
1.508	Mn_2AlB_2	$Cmmm$ (65)	C_cmcm (63.466)	$mmm1'$	×	×
1.509	$Pd_{2.87}Mn_{0.88}$	$I4/mmm$ (139)	P_A2_1/c (14.83)	$2/m1'$	×	×
1.510	$TbNi_2Ge_2$	$I4/mmm$ (139)	P_c4/mcc (124.360)	$4/mmm1'$	×	×
1.511	$TbNi_2Si_2$	$I4/mmm$ (139)	C_Amca (64.480)	$mmm1'$	×	×
1.512	$TbCo_2Si_2$	$I4/mmm$ (139)	P_I4/mnc (128.410)	$4/mmm1'$	×	×
1.513	$HoCo_2Si_2$	$I4/mmm$ (139)	P_I4/mnc (128.410)	$4/mmm1'$	×	×
1.514	$HoCo_2Si_2$	$I4/mmm$ (139)	P_I4/mnc (128.410)	$4/mmm1'$	×	×
1.515	$ErCo_2Si_2$	$I4/mmm$ (139)	P_A2_1/c (14.83)	$2/m1'$	×	×
1.516	$ErCo_2Si_2$	$I4/mmm$ (139)	P_Innm (58.404)	$mmm1'$	×	×
1.517	$DyBe_{13}$	$Fm\bar{3}c$ (226)	C_A222_1 (20.37)	$2221'$	G-wP	×
1.518	$TbBe_{13}$	$Fm\bar{3}c$ (226)	C_A222_1 (20.37)	$2221'$	G-wP	×
1.519	$CoSO_4$	$Cmcm$ (63)	P_Cbcn (60.431)	$mmm1'$	×	×
1.520	$NiSO_4$	$Cmcm$ (63)	P_Cbcn (60.431)	$mmm1'$	×	×
1.521	$FeSO_4$	$Cmcm$ (63)	P_Cbcn (60.431)	$mmm1'$	×	×
1.522	$CrVO_4$	$Cmcm$ (63)	$P\bar{1}$ (2.4)	$\bar{1}$	×	✓
1.523	VPO_4	$Cmcm$ (63)	P_cnma (62.452)	$mmm1'$	×	×
1.524	$InMnO_3$	$P6_3cm$ (185)	P_c31c (159.64)	$3m1'$	G-woP	×
1.525	$InMnO_3$	$P6_3cm$ (185)	P_c31m (157.56)	$3m1'$	G-woP	×
1.526	$LiCoF_4$	$P2_1/c$ (14)	P_a2_1/c (14.80)	$2/m1'$	×	×
1.527	$CsNiF_3$	$P6_3/mmc$ (194)	P_Bnnm (58.402)	$mmm1'$	×	×
1.528	$Bi_2Fe_4O_9$	$Pbam$ (55)	C_a2/m (12.64)	$2/m1'$	×	×
1.529	MnBi6Te10	$R\bar{3}m$ (166)	$R_I\bar{3}c$ (167.108)	$\bar{3}m1'$	×	×
1.530	CeC_2	$I4/mmm$ (139)	P_I4/mnc (128.410)	$4/mmm1'$	×	×
1.531	PrC_2	$I4/mmm$ (139)	P_I4/mnc (128.410)	$4/mmm1'$	×	×
1.532	NdC_2	$I4/mmm$ (139)	P_I4/mnc (128.410)	$4/mmm1'$	×	×
1.533	TbC_2	$I4/mmm$ (139)	P_c222_1 (17.12)	$2221'$	G-wP	×
1.534	HoC_2	$I4/mmm$ (139)	P_amma (51.298)	$mmm1'$	×	×

Continued on next page

Suppl. Tab. XI – continued from previous page

BCS-ID	Formula	Parent	MSG	MPG	SHG type	LMO
1.535	UPd_2Ge_2	$I4/mmm$ (139)	P_c4/ncc (130.432)	$4/mmm1'$	×	×
1.536	UPd_2Si_2	$I4/mmm$ (139)	P_I4/mnc (128.410)	$4/mmm1'$	×	×
1.537	URh_2Si_2	$I4/mmm$ (139)	P_I4/mnc (128.410)	$4/mmm1'$	×	×
1.538	Ba_2MnTeO_6	$R\bar{3}m$ (166)	P_A2_1/c (14.83)	$2/m1'$	×	×
1.539	KMnP	$P4/nmm$ (129)	P_c4_2/ncm (138.528)	$4/mmm1'$	×	×
1.540	KMnP	$P4/nmm$ (129)	P_c4_2/ncm (138.528)	$4/mmm1'$	×	×
1.541	RbMnP	$P4/nmm$ (129)	P_c4_2/ncm (138.528)	$4/mmm1'$	×	×
1.542	RbMnP	$P4/nmm$ (129)	P_c4_2/ncm (138.528)	$4/mmm1'$	×	×
1.543	RbMnAs	$P4/nmm$ (129)	P_c4_2/ncm (138.528)	$4/mmm1'$	×	×
1.544	RbMnAs	$P4/nmm$ (129)	P_c4_2/ncm (138.528)	$4/mmm1'$	×	×
1.545	RbMnBi	$P4/nmm$ (129)	P_c4_2/ncm (138.528)	$4/mmm1'$	×	×
1.546	CsMnBi	$P4/nmm$ (129)	P_c4_2/ncm (138.528)	$4/mmm1'$	×	×
1.547	CsMnP	$P4/nmm$ (129)	P_c4_2/ncm (138.528)	$4/mmm1'$	×	×
1.548	CsMnP	$P4/nmm$ (129)	P_c4_2/ncm (138.528)	$4/mmm1'$	×	×
1.549	U_2Ni_2In	$P4/mbm$ (127)	P_c4/mnc (128.408)	$4/mmm1'$	×	×
1.550	LiMnAs	$P4/nmm$ (129)	P_c4_2/ncm (138.528)	$4/mmm1'$	×	×
1.551	LiMnAs	$P4/nmm$ (129)	P_c4_2/ncm (138.528)	$4/mmm1'$	×	×
1.552	LiMnAs	$P4/nmm$ (129)	P_c4_2/ncm (138.528)	$4/mmm1'$	×	×
1.553	KMnAs	$P4/nmm$ (129)	P_c4_2/ncm (138.528)	$4/mmm1'$	×	×
1.554	KMnAs	$P4/nmm$ (129)	P_c4_2/ncm (138.528)	$4/mmm1'$	×	×
1.555	Mn_3B_4	$Immm$ (71)	P_Innm (58.404)	$mmm1'$	×	×
1.556	$FeSn_2$	$I4/mcm$ (140)	P_Ibcn (60.432)	$mmm1'$	×	×
1.557	$FeGe_2$	$I4/mcm$ (140)	P_Ibcn (60.432)	$mmm1'$	×	×
1.558	$MnSn_2$	$I4/mcm$ (140)	C_Acca (68.520)	$mmm1'$	×	×
1.559	$MnSn_2$	$I4/mcm$ (140)	C_cccm (66.498)	$mmm1'$	×	×
1.560	$GeNi_2O_4$	$Fd\bar{3}m$ (227)	C_c2/m (12.63)	$2/m1'$	×	×
1.561	$GeNi_2O_4$	$Fd\bar{3}m$ (227)	C_cm (8.35)	$m1'$	G-wP	×
1.562	$GeNi_2O_4$	$Fd\bar{3}m$ (227)	C_c2 (5.16)	$21'$	G-wP	×
1.563	$GeNi_2O_4$	$Fd\bar{3}m$ (227)	C_cm (8.35)	$m1'$	G-wP	×
1.564	$GeCo_2O_4$	$Fd\bar{3}m$ (227)	C_c2 (5.16)	$21'$	G-wP	×
1.565	Pb_2CoOsO_6	$P2_1/n$ (14)	P_ac (7.27)	$m1'$	G-wP	×
1.566	Ba_2YbRuO_6	$Fm\bar{3}m$ (225)	P_I4/mnc (128.410)	$4/mmm1'$	×	×
1.567	Ba_2TmRuO_6	$Fm\bar{3}m$ (225)	P_I4/mnc (128.410)	$4/mmm1'$	×	×
1.568	$GdCu_2Si_2$	$I4/mmm$ (139)	C_c2/m (12.63)	$2/m1'$	×	×
1.569	$SrRu_2O_6$	$P\bar{3}1m$ (162)	$P_c\bar{3}1m$ (162.78)	$\bar{3}m1'$	×	×
1.570	La_3OsO_7	$Cmcm$ (63)	P_a2_1/m (11.55)	$2/m1'$	×	×
1.571	La_3OsO_7	$Cmcm$ (63)	P_a2_1/m (11.55)	$2/m1'$	×	×
1.572	$La_{2.8}Ca_{0.2}OsO_7$	$Cmcm$ (63)	P_a2_1/m (11.55)	$2/m1'$	×	×
1.573	$FeSO_4$	$Pbnm$ (62)	P_c2_1/c (14.82)	$2/m1'$	×	×
1.574	NdBiPt	$F\bar{4}3m$ (216)	$P_I\bar{4}n2$ (118.314)	$\bar{4}2m1'$	G-woP	×
1.575	ErRh	$Pm\bar{3}m$ (221)	P_amma (51.298)	$mmm1'$	×	×
1.576	Yb_2O_2S	$P\bar{3}m1$ (164)	C_c2/m (12.63)	$2/m1'$	×	×
1.577	$SrNd_2O_4$	$Pnam$ (62)	P_a2_1/c (14.80)	$2/m1'$	×	×
1.578	$KErSe_2$	$R\bar{3}m$ (166)	C_c2/m (12.63)	$2/m1'$	×	×
1.579	$NiTiO_3$	$R\bar{3}$ (148)	$P_S\bar{1}$ (2.7)	$\bar{1}1'$	×	×
1.580	$NiTiO_3$	$R\bar{3}$ (148)	$P_S\bar{1}$ (2.7)	$\bar{1}1'$	×	×
1.581	$FeTiO_3$	$R\bar{3}$ (148)	$R_I\bar{3}$ (148.20)	$\bar{3}1'$	×	×
1.582	$Fe_{0.945}O$	$Fm\bar{3}m$ (225)	$R_I\bar{3}c$ (167.108)	$\bar{3}m1'$	×	×
1.583	$La_{1.5}Ca_{0.5}CoO_4$	$Cmm2$ (35)	P_cc (7.28)	$m1'$	G-woP	×
1.584	PrFeAsO	$Cmme$ (67)	P_Bcca (54.350)	$mmm1'$	×	×
1.585	PrFeAsO	$Cmme$ (67)	P_Bcca (54.350)	$mmm1'$	×	×

Continued on next page

Suppl. Tab. XI – continued from previous page

BCS-ID	Formula	Parent	MSG	MPG	SHG type	LMO
1.586	PrFeAsO	$Cmme$ (67)	P_Acc2 (27.85)	$mm21'$	G-wP	×
1.587	NdFeAsO	$Cmme$ (67)	P_A2/c (13.73)	$2/m1'$	×	×
1.588	NdFeAsO	$Cmme$ (67)	I_cbca (73.553)	$mmm1'$	×	×
1.589	$Fe_{0.967}Nb_3S_6$	$P6_322$ (182)	$P_c2_12_12$ (18.21)	$2221'$	G-woP	×
1.590	$Pb_{0.8}Bi_{0.2}Fe_{0.728}W_{0.264}O_3$	$Pm\bar{3}m$ (221)	I_c4/mcm (140.550)	$4/mmm1'$	×	×
1.591	$Pb_{0.7}Bi_{0.3}Fe_{0.762}W_{0.231}O_3$	$Pm\bar{3}m$ (221)	I_c4/mcm (140.550)	$4/mmm1'$	×	×
1.592	Pb_2NiOsO_6	$P2_1/n$ (14)	P_ac (7.27)	$m1'$	G-wP	×
1.593	BaCoSO	$Cmcm$ (63)	P_abcm (57.386)	$mmm1'$	×	×
1.594	BaCoSO	$Cmcm$ (63)	P_abcm (57.386)	$mmm1'$	×	×
1.595	CaCoSO	$P6_3mc$ (186)	C_cc (9.40)	$m1'$	G-woP	×
1.596	$TbCuSb_2$	$P4/nmm$ (129)	$P_S\bar{1}$ (2.7)	$\bar{1}1'$	×	×
1.597	$TbCuSb_2$	$P4/nmm$ (129)	P_a2_1/m (11.55)	$2/m1'$	×	×
1.598	$CeIr(In_{0.97}Cd_{0.03})_5$	$P4/mmm$ (123)	I_c4/mcm (140.550)	$4/mmm1'$	×	×
1.599	$DyMn_2O_5$	$Pbam$ (55)	P_cc (7.28)	$m1'$	G-wP	×
1.600	$Bi_4Fe_5O_{13}F$	$P4_2/mbc$ (135)	P_C42/n (86.73)	$4/m1'$	×	×
1.601	$Bi_4Fe_5O_{13}F$	$P4_2/mbc$ (135)	P_C42/n (86.73)	$4/m1'$	×	×
1.602	$Bi_4Fe_5O_{13}F$	$P4_2/mbc$ (135)	P_C42/n (86.73)	$4/m1'$	×	×
1.603	$Bi_4Fe_5O_{13}F$	$P4_2/mbc$ (135)	P_C42/n (86.73)	$4/m1'$	×	×
1.604	$Bi_4Fe_5O_{13}F$	$P4_2/mbc$ (135)	P_C42/n (86.73)	$4/m1'$	×	×
1.605	$Bi_4Fe_5O_{13}F$	$P4_2/mbc$ (135)	P_C42/n (86.73)	$4/m1'$	×	×
1.606	$Bi_4Fe_5O_{13}F$	$P4_2/mbc$ (135)	P_C42/n (86.73)	$4/m1'$	×	×
1.607	$Bi_4Fe_5O_{13}F$	$P4_2/mbc$ (135)	P_C42/n (86.73)	$4/m1'$	×	×
1.608	$Bi_4Fe_5O_{13}F$	$P4_2/mbc$ (135)	P_C42/n (86.73)	$4/m1'$	×	×
1.609	$Bi_4Fe_5O_{13}F$	$P4_2/mbc$ (135)	P_C42/n (86.73)	$4/m1'$	×	×
1.610	$Bi_4Fe_5O_{13}F$	$P4_2/mbc$ (135)	P_C42/n (86.73)	$4/m1'$	×	×
1.611	$Bi_4Fe_5O_{13}F$	$P4_2/mbc$ (135)	P_C42/n (86.73)	$4/m1'$	×	×
1.612	$Bi_4Fe_5O_{13}F$	$P4_2/mbc$ (135)	P_C42/n (86.73)	$4/m1'$	×	×
1.613	$Bi_4Fe_5O_{13}F$	$P4_2/mbc$ (135)	P_C42/n (86.73)	$4/m1'$	×	×
1.614	$Bi_4Fe_5O_{13}F$	$P4_2/mbc$ (135)	P_C42/n (86.73)	$4/m1'$	×	×
1.615	$Bi_4Fe_5O_{13}F$	$P4_2/mbc$ (135)	P_C42/n (86.73)	$4/m1'$	×	×
1.616	$Bi_4Fe_5O_{13}F$	$P4_2/mbc$ (135)	P_C42/n (86.73)	$4/m1'$	×	×
1.617	$LiFe(MoO_4)_2$	$P\bar{1}$ (2)	$P_S\bar{1}$ (2.7)	$\bar{1}1'$	×	×
1.618	CoO	$Fm\bar{3}m$ (225)	C_c2/c (15.90)	$2/m1'$	×	×
1.619	MnS	$Fm\bar{3}m$ (225)	C_c2/m (12.63)	$2/m1'$	×	×
1.620	$NdCu_2$	$Imma$ (74)	P_Inma (62.456)	$mmm1'$	×	×
1.621	$La(Fe_{0.91}Al_{0.09})_{13}$	$Fm\bar{3}c$ (226)	P_I4/mcc (124.362)	$4/mmm1'$	×	×
1.622	$CoGeO_3$	$C2/c$ (15)	P_C2_1/c (14.84)	$2/m1'$	×	×
1.623	$EuMg_2Bi_2$	$P\bar{3}m1$ (164)	C_c2/m (12.63)	$2/m1'$	×	×
1.624	$EuSn_2P_2$	$R\bar{3}m$ (166)	C_c2/m (12.63)	$2/m1'$	×	×
1.625	$Sr_2Fe_3S_2O_3$	$Pbam$ (55)	P_bnma (62.451)	$mmm1'$	×	×
1.626	$Sr_2Fe_3Se_2O_3$	$Pbam$ (55)	C_amc2_1 (36.178)	$mm21'$	G-wP	×
1.627	$KCeS_2$	$R\bar{3}m$ (166)	C_c2/c (15.90)	$2/m1'$	×	×
1.628	$PrMnSi_2$	$Cmcm$ (63)	P_Bnna (52.318)	$mmm1'$	×	×
1.629	FeGe	$P6/mmm$ (191)	P_c6/mcc (192.252)	$6/mmm1'$	×	×
1.630	$LuMn_6Sn_6$	$P6/mmm$ (191)	C_cmcm (63.466)	$mmm1'$	×	×
1.631	YMn_6Ge_6	$P6/mmm$ (191)	P_c6/mcc (192.252)	$6/mmm1'$	×	×
1.632	$ErFe_6Ge_6$	$Immm$ (71)	P_Innn (48.264)	$mmm1'$	×	×
1.633	YFe_6Sn_6	$Immm$ (71)	P_Innn (48.264)	$mmm1'$	×	×
1.634	YFe_6Ge_6	$Cmcm$ (63)	P_Bnna (52.318)	$mmm1'$	×	×
1.635	$ErFe_2Si_2$	$I4/mmm$ (139)	P_anma (62.450)	$mmm1'$	×	×
1.636	$ErMn_2Si_2$	$I4/mmm$ (139)	P_I4/nnc (126.386)	$4/mmm1'$	×	×

Continued on next page

Suppl. Tab. XI – continued from previous page

BCS-ID	Formula	Parent	MSG	MPG	SHG type	LMO
1.637	$ErMn_2Si_2$	$I4/mmm$ (139)	P_I4/nnc (126.386)	$4/mmm1'$	×	×
1.638	$ErMn_2Ge_2$	$I4/mmm$ (139)	P_I4/nnc (126.386)	$4/mmm1'$	×	×
1.639	$ErMn_2Ge_2$	$I4/mmm$ (139)	P_I4/nnc (126.386)	$4/mmm1'$	×	×
1.640	$ErMn_2Ge_2$	$I4/mmm$ (139)	P_I4/nnc (126.386)	$4/mmm1'$	×	×
1.641	$Ba_2FeSi_2O_7$	$P\bar{4}2_1m$ (113)	C_cmc2_1 (36.177)	$mm21'$	G-woP	×
1.642	$TlFeS_2$	$C2/m$ (12)	C_c2/m (12.63)	$2/m1'$	×	×
1.643	$DyOCl$	$P4/nmm$ (129)	P_anma (62.450)	$mmm1'$	×	×
1.644	$EuSn_2As_2$	$R\bar{3}m$ (166)	C_c2/m (12.63)	$2/m1'$	×	×
1.645	$Na_2Co_2TeO_6$	$P6_322$ (182)	$P_C2_12_12_1$ (19.29)	$2221'$	G-woP	×
1.646	$Na_2Ni_2TeO_6$	$P6_3/mcm$ (193)	I_amm2 (44.234)	$mm21'$	G-wP	×
1.647	$Na_{2.4}Ni_2TeO_6$	$P6_3/mcm$ (193)	P_Anma (62.453)	$mmm1'$	×	×
1.648	Nd_2O_3	$P\bar{3}m1$ (164)	C_c2/m (12.63)	$2/m1'$	×	×
1.649	Sr_3ZnIrO_6	$R\bar{3}c$ (167)	P_C2/c (13.74)	$2/m1'$	×	×
1.650	$DyBaCuO_5$	$Pnma$ (62)	P_a2_1/c (14.80)	$2/m1'$	×	×
1.651	$HoBaCuO_5$	$Pnma$ (62)	P_a2_1/c (14.80)	$2/m1'$	×	×
1.652	$Tb_2Ni_{1.78}In$	$P/4mbm$ (127)	C_amca (64.479)	$mmm1'$	×	×
1.653	$FeWO_4$	$P2/c$ (13)	P_a2/c (13.70)	$2/m1'$	×	×
1.654	$NiNb_2O_6$	$Pbcn$ (60)	P_b2_1/c (14.81)	$2/m1'$	×	×
1.655	$FeNb_2O_6$	$Pbcn$ (60)	$P_c2_12_12_1$ (19.28)	$2221'$	G-wP	×
1.656	$CoNb_2O_6$	$Pbcn$ (60)	P_a2_1/c (14.80)	$2/m1'$	×	×
1.657	$LuNiO_3$	$P2_1/n$ (14)	P_a2_1 (4.10)	$21'$	G-wP	×
1.658	$DyGa_3$	$R\bar{3}m$ (166)	C_c2/c (15.90)	$2/m1'$	×	×
1.659	$MnCl_2(CO(NH_2)_2)_2$	$Iba2$ (45)	P_Ica2_1 (29.110)	$mm21'$	G-woP	×
1.660	$FePb_4Sb_6S_{14}$	$P2_1/c$ (14)	P_a2_1/c (14.80)	$2/m1'$	×	×
1.661	La_2NiIrO_6	$P2_1/n$ (14)	$P_S\bar{1}$ (2.7)	$\bar{1}1'$	×	×
1.662	La_2NiIrO_6	$P2_1/n$ (14)	$P_S\bar{1}$ (2.7)	$\bar{1}1'$	×	×
1.663	Tb_2Ni_2In	$Cmmm$ (65)	C_a2/m (12.64)	$2/m1'$	×	×
2.1	$EuFe_2As_2$	$I4/mmm$ (139)	P_Cbca (61.439)	$mmm1'$	×	×
2.2	$Sr_2F_2Fe_2OS_2$	$I4/mmm$ (139)	C_a2/m (12.64)	$2/m1'$	×	×
2.3	$HoNiO_3$	$P2_1/n$ (14)	$P2_1$ (4.7)	2	O-wP	✓
2.4	$Eu(Fe_{0.82}Co_{0.18})As_2$	$I4/mmm$ (139)	$Cmm'm'$ (65.486)	$m'm'm$	×	✓
2.5	Mn_3CuN	$Pm\bar{3}m$ (221)	$P4/n$ (85.59)	$4/m$	×	✓
2.6	Nd_2CuO_4	$I4/mmm$ (139)	P_C4_2/nnm (134.481)	$4/mmm1'$	×	×
2.7	Sm_2CuO_4	$I4/mmm$ (139)	P_C4_2/ncm (138.529)	$4/mmm1'$	×	×
2.8	$SrHo_2O_4$	$Pnam$ (62)	$P2_1/c'$ (14.78)	$2/m'$	PT-wP	×
2.9	$Ca_3CuNi_2(PO_4)_4$	$C2/c$ (15)	C_a2/c (15.91)	$2/m1'$	×	×
2.1	HoP	$Fm\bar{3}m$ (225)	$C2'/c'$ (15.89)	$2'/m'$	×	✓
2.11	$TbMg$	$Pm\bar{3}m$ (221)	$Pmm'a'$ (51.295)	$m'm'm$	×	✓
2.12	$TbMg$	$Pm\bar{3}m$ (221)	$Pc'cm'$ (49.270)	$m'm'm$	×	✓
2.13	UP	$Fm\bar{3}m$ (225)	P_C4_2/nnm (134.481)	$4/mmm1'$	×	×
2.14	$NdMg$	$Pm\bar{3}m$ (221)	P_C4/nbm (125.373)	$4/mmm1'$	×	×
2.15	$Mn_3Ni_20P_6$	$Fm\bar{3}m$ (225)	$Cmm'm'$ (65.486)	$m'm'm$	×	✓
2.16	Ce_2PdGe_3	$P4_2/mmc$ (131)	Pm' (6.20)	m'	BW-wP	✓
2.17	$Pb_2Mn_{0.6}Co_{0.4}WO_6$	$Pmcn$ (62)	$Pm'c2_1'$ (26.68)	$m'm2'$	BW-wP	✓
2.18	Sc_2NiMnO_6	$P2_1/c$ (14)	$P_S\bar{1}$ (2.7)	$\bar{1}1'$	×	×
2.19	Mn_3ZnC	$Pm\bar{3}m$ (221)	$I4/mm'm'$ (139.537)	$4/mm'm'$	×	✓
2.20	UAs	$Fm\bar{3}m$ (225)	P_C4_2/nnm (134.481)	$4/mmm1'$	×	×
2.21	$TbOOH$	$P2_1/m$ (11)	$P2_1/c'$ (14.78)	$2/m'$	PT-wP	×
2.22	$FeTa_2O_6$	$P4_2/mnm$ (136)	I_c4_1/a (88.86)	$4/m1'$	×	×
2.23	$Sr_2CoO_2Ag_2Se_2$	$I4/mmm$ (139)	P_C42/n (86.73)	$4/m1'$	×	×
2.24	$Ba_2CoO_2Ag_2Se_2$	$I4/mmm$ (139)	P_C42/n (86.73)	$4/m1'$	×	×

Continued on next page

Suppl. Tab. XI – continued from previous page

BCS-ID	Formula	Parent	MSG	MPG	SHG type	LMO
2.25	Sr_2CoOsO_6	$I2/m$ (12)	$P_S\bar{1}$ (2.7)	$\bar{1}1'$	×	×
2.26	$PrCo_2P_2$	$I4/mmm$ (139)	$P4/mm'm'$ (123.345)	$4/mm'm'$	×	✓
2.27	$Sr_2Mn_3Sb_2O_2$	$I4/mmm$ (139)	$Cm'cm$ (63.459)	$m'mm$	PT-wP	×
2.28	$NpNiGa_5$	$P4/mmm$ (123)	$Imm'a'$ (74.559)	$m'm'm$	×	✓
2.29	Mn_3O_4	$I4_1/amd$ (141)	$Pb'c'n$ (60.422)	$m'm'm$	×	✓
2.30	$CeRh_2Si_2$	$I4/mmm$ (139)	P_Bcca (54.350)	$mmm1'$	×	×
2.31	Mn_3ZnN	$Pm\bar{3}m$ (221)	P_Ibcn (60.432)	$mmm1'$	×	×
2.32	$Dy_3Ru_4Al_{12}$	$P6_3/mmc$ (194)	$P\bar{3}c'1$ (165.95)	$\bar{3}m'$	×	✓
2.33	$Na_2Mn_3Se_4$	$C2/m$ (12)	$P_S\bar{1}$ (2.7)	$\bar{1}1'$	×	×
2.34	$La_{0.25}Pr_{0.75}Co_2P_2$	$I4/mmm$ (139)	$C2'/m'$ (12.62)	$2'/m'$	×	✓
2.35	$CrSe$	$P6_3/mmc$ (194)	$P31m'$ (157.55)	$3m'$	BW-wP	✓
2.36	$TbGe_3$	$Cmcm$ (63)	P_cnma (62.452)	$mmm1'$	×	×
2.37	$La_8Cu_7O_{19}$	$C2/c$ (15)	$P_S\bar{1}$ (2.7)	$\bar{1}1'$	×	×
2.38	Pb_2MnWO_6	$Pmc2_1$ (26)	$Pmn2_1$ (31.123)	$mm2$	O-woP	×
2.39	$LaCaFeO_4$	$I4/mmm$ (139)	P_C4_2/ncm (138.529)	$4/mmm1'$	×	×
2.40	$LaBaFeO_4$	$I4/mmm$ (139)	P_C4_2/ncm (138.529)	$4/mmm1'$	×	×
2.41	$LaSrFeO_4$	$I4/mmm$ (139)	P_C4_2/ncm (138.529)	$4/mmm1'$	×	×
2.42	$LaSrFeO_4$	$I4/mmm$ (139)	P_C4_2/nnm (134.481)	$4/mmm1'$	×	×
2.43	Fe_2MnBO_5	$Pbam$ (55)	$Pb'am'$ (55.358)	$m'm'm$	×	✓
2.44	$KCuMnS_2$	$I4/mmm$ (139)	P_C4/mmm (123.349)	$4/mmm1'$	×	×
2.45	$Pb_2BaCuFeO_5Br$	$P4/mmm$ (123)	P_C2 (3.6)	$21'$	G-wP	×
2.46	$Pb_2BaCuFeO_5Cl$	$P4/mmm$ (123)	P_C2 (3.6)	$21'$	G-wP	×
2.47	$Y_2SrCuFeO_{6.5}$	$Ibam$ (72)	$Pc'c'n$ (56.369)	$m'm'm$	×	✓
2.48	Pr_2CuO_4	$I4/mmm$ (139)	P_C4_2/nnm (134.481)	$4/mmm1'$	×	×
2.49	$La_2O_2Fe_2OSe_2$	$I4/mmm$ (139)	C_a2/m (12.64)	$2/m1'$	×	×
2.50	$EuMnBi_2$	$I4/mmm$ (139)	$P4_2'/m'm'c$ (131.440)	$4'/m'm'm$	PT-wP	×
2.51	$EuMnBi_2$	$I4/mmm$ (139)	$Pm'n'2_1$ (31.127)	$m'm'2$	BW-wP	✓
2.52	Mn_3O_4	$I4_1/amd$ (141)	Pc' (7.26)	m'	BW-wP	✓
2.53	$Ba_2Mn_3Sb_2O_2$	$I4/mmm$ (139)	$Cm'ma$ (67.503)	$m'mm$	PT-wP	×
2.54	$Sr_2Cr_3As_2O_2$	$I4/mmm$ (139)	P_C2_1/c (14.84)	$2/m1'$	×	×
2.55	$Sr_2Fe_3Se_2O_3$	$Pbam$ (55)	C_cc (9.40)	$m1'$	G-wP	×
2.56	$La_2O_2Fe_2OS_2$	$I4/mmm$ (139)	C_a2/m (12.64)	$2/m1'$	×	×
2.57	$TbMn_2Si_2$	$I4/mmm$ (139)	$Pmm'n'$ (59.410)	$m'm'm$	×	✓
2.58	$La_{0.73}Tb_{0.27}Mn_2Si_2$	$I4/mmm$ (139)	$Pnnm'$ (58.396)	$m'mm$	PT-wP	×
2.59	Mn_3As_2	$C2/m$ (12)	$C2/c$ (15.85)	$2/m$	×	✓
2.60	$NdMn_2Si_2$	$I4/mmm$ (139)	$Pmm'n'$ (59.410)	$m'm'm$	×	✓
2.61	$Fe_3F_8(H_2O)_2$	$C2/m$ (12)	$C2'/m'$ (12.62)	$2'/m'$	×	✓
2.62	$TbCrO_3$	$Pbnm$ (62)	$Pm'n'2_1$ (31.127)	$m'm'2$	BW-wP	✓
2.63	$DyCrO_3$	$Pbnm$ (62)	$P2_1'/m'$ (11.54)	$2'/m'$	×	✓
2.64	$DyCrO_3$	$Pbnm$ (62)	$P2_1'/m'$ (11.54)	$2'/m'$	×	✓
2.65	UPd_2Si_2	$I4/mmm$ (139)	$P4/mm'm'$ (123.345)	$4/mm'm'$	×	✓
2.66	$FeSn_2$	$I4/mcm$ (140)	$Cc'ca$ (68.513)	$m'mm$	PT-wP	×
2.67	$FeSn_2$	$I4/mcm$ (140)	P_Cbcn (60.431)	$mmm1'$	×	×
2.68	$FeGe_2$	$I4/mcm$ (140)	$Pc'cn$ (56.367)	$m'mm$	PT-wP	×
2.69	$La_{0.5}Ca_{0.5}MnO_3$	$Pnma$ (62)	P_a2_1/m (11.55)	$2/m1'$	×	×
2.70	$GdMg$	$Pm\bar{3}m$ (221)	$C2'/c'$ (15.89)	$2'/m'$	×	✓
2.71	$HoRh$	$Pm\bar{3}m$ (221)	P_C2_1/m (11.57)	$2/m1'$	×	×
2.72	VNb_3S_6	$P6_322$ (182)	$C2'2'2_1$ (20.33)	$2'2'2$	BW-woP	✓
2.73	$BaNd_2ZnO_5$	$I4/mcm$ (140)	P_C4/ncc (130.433)	$4/mmm1'$	×	×
2.74	$BaDy_2O_4$	$Pnma$ (62)	$P2_1'$ (4.9)	$2'$	BW-wP	✓
2.75	$Sr_2Fe_3S_2O_3$	$Pbam$ (55)	P_A2_1/c (14.83)	$2/m1'$	×	×

Continued on next page

Suppl. Tab. XI – continued from previous page

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

[1] S. N. Rashkeev, W. R. L. Lambrecht, and B. Segall, Phys. Rev. B **57**, 3905 (1998).
[2] C. Wang, X. Liu, L. Kang, B.-L. Gu, Y. Xu, and W. Duan, Phys. Rev. B **96**, 115147 (2017).
[3] H. Chen, M. Ye, N. Zou, B.-L. Gu, Y. Xu, and W. Duan, Phys. Rev. B **105**, 075123 (2022).
[4] D. B. Litvin, Magnetic Group Tables 1-, 2- and 3-Dimensional Magnetic Subperiodic Groups and Magnetic Space Groups (Reviewed by the IUCr Commission on Magnetic Structures, 2013).
[5] C. J. Bardley and A. P. Cracknell, The mathematical theory of symmetry in solids: representation theory for point groups and spa (Oxford University Press, 2010).
[6] R. Tao, Group Theory in Physics (in Chinese) (Shanghai Scientific & Technical Publishers, 1986).
[7] R. R. Birss, Symmetry and magnetism (North-Holland Publishing Company, 1964).
[8] S. Y. Litvin and D. B. Litvin, Acta Crystallogr. A **47**, 290 (1991).
[9] S. V. Gallego, J. Etxebarria, L. Elcoro, E. S. Tasci, and J. M. Perez-Mato, Acta Crystallogr A Found Adv **75**, 438 (2019).
[10] J. Železný, H. Gao, A. Manchon, F. Freimuth, Y. Mokrousov, J. Zemen, J. Mašek, J. Sinova, and T. Jungwirth, Phys. Rev. B **95**, 014403 (2017).
[11] R. W. Boyd, Nonlinear optics (Academic press, 2010).
[12] S. Shi, G. Chen, W. Zhao, and L. Jifang, Nonlinear optics (in Chinese) (Xidian University press, 2012).
[13] A. P. Cracknell, Phys. Rev. B **7**, 2145 (1973).
[14] A. Kirilyuk, J. Phys. D: Appl. Phys. **35**, R189 (2002).
[15] H. Grimmer, Acta Crystallogr. A **49**, 763 (1993).
[16] T. Hahn, U. Shmueli, and J. W. Arthur, International tables for crystallography, Vol. 1 (Reidel Dordrecht, 1983).
[17] C. L. Kane and E. J. Mele, Phys. Rev. Lett. **95**, 146802 (2005).
[18] X. Li, T. Cao, Q. Niu, J. Shi, and J. Feng, P. Natl. Acad. Sci. USA **110**, 3738 (2013).

[19] W. Y. Tong, S. J. Gong, X. Wan, and C. G. Duan, Nat. Commun. **7**, 13612 (2016).
[20] Z. Sun, Y. Yi, T. Song, G. Clark, B. Huang, Y. Shan, S. Wu, D. Huang, C. Gao, Z. Chen, M. McGuire, T. Cao, D. Xiao, W. T. Liu, W. Yao, X. Xu, and S. Wu, Nature **572**, 497 (2019).
[21] V. K. Gudelli and G.-Y. Guo, Chin. J. Phys. **68**, 896 (2020).
[22] W. Song, R. Fei, L. Zhu, and L. Yang, Phys. Rev. B **102**, 045411 (2020).
[23] H. Chu, C. J. Roh, J. O. Island, C. Li, S. Lee, J. Chen, J.-G. Park, A. F. Young, J. S. Lee, and D. Hsieh, Phys. Rev. Lett. **124**, 027601 (2020).
[24] Z. Ni, A. V. Haglund, H. Wang, B. Xu, C. Bernhard, D. G. Mandrus, X. Qian, E. J. Mele, C. L. Kane, and L. Wu, Nat. Nanotechnol. **16**, 782 (2021).
[25] R. Fei, W. Song, and L. Yang, Phys. Rev. B **102**, 035440 (2020).
[26] K. Lee, A. H. Dismukes, E. J. Telford, R. A. Wiscons, J. Wang, X. Xu, C. Nuckolls, C. R. Dean, X. Roy, and X. Zhu, Nano Lett. **21**, 3511 (2021).
[27] N. Sivadas, S. Okamoto, and D. Xiao, Phys. Rev. Lett. **117**, 267203 (2016).
[28] A. Taghizadeh, F. Hipolito, and T. G. Pedersen, Phys. Rev. B **96**, 195413 (2017).
[29] Y. Deng, Y. Yu, Y. Song, J. Zhang, N. Z. Wang, Z. Sun, Y. Yi, Y. Z. Wu, S. Wu, J. Zhu, J. Wang, X. H. Chen, and Y. Zhang, Nature **563**, 94 (2018).
[30] R.-C. Xiao, Y. Gao, H. Jiang, W. Gan, C. Zhang, and H. Li, npj Comput. Mater. **8**, 138 (2022).
[31] A. Muñoz, J. A. Alonso, M. J. Martínez-Lope, M. T. Casáis, J. L. Martínez, and M. T. Fernández-Díaz, Phys. Rev. B **62**, 9498 (2000).
[32] P. Liu, J. Li, J. Han, X. Wan, and Q. Liu, Phys. Rev. X **12**, 021016 (2022).
[33] Y. Zhang, J. Železný, Y. Sun, J. van den Brink, and B. Yan, New J. Phys. **20**, 073028 (2018).
[34] M. T. Suzuki, T. Koretsune, M. Ochi, and R. Arita, Phys. Rev. B **95**, 094406 (2017).
[35] R.-C. Xiao, D.-F. Shao, Y.-H. Li, and H. Jiang, npj Quantum Mater. **6**, 35 (2021).
[36] H. Xu, H. Wang, J. Zhou, and J. Li, Nat. Commun. **12**, 4330 (2021).