Supplemental Materials for "Magnetic Structures Database from Symmetry-aided High-Throughput Calculations"

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A. Irreducible-Representation Basis-Vector Strategy of Initial Magnetic Structures

Most magnetic phase transitions are continuous and can be described within the Landau framework [1]. From a symmetry perspective, the ordered phase is described by magnetic space groups (MSGs) that are subgroups of the parent crystallographic space group. However, the subgroup landscape is typically vast: a given parent space group admits many magnetic subgroups associated with many irreducible representations (irreps).

To systematically reduce this space, we take the magnetic moments $\boldsymbol{\mu}$ on the magnetic Wyckoff positions as a basis. For a crystal with N magnetic atoms in the crystallographic unit cell (at $\mathbf{q} = 0$), the $3N$ components of the local moments $\boldsymbol{\mu} = (m_{1x}, m_{1y}, m_{1z}, \ldots, m_{Nx}, m_{Ny}, m_{Nz})$ span a representation Γ_{mag} of the parent space group, which is in general reducible and can be decomposed into irreducible representations as

$$\Gamma_{\mathrm{mag}} = \sum_{\oplus i} n_i \, \Gamma_i(j). \tag{1}$$

Here we adopt the Cracknell–Davies–Miller–Love (CDML) notation [2], where the subscript i labels distinct irreducible representations, j denotes the irrep dimensionality, and the prefactor n_i specifies the multiplicity.

Within Landau theory, a continuous magnetic transition is driven by the instability of a single irreducible representation in Eq. (1). Consequently, only the MSGs compatible with this unstable irrep need to be considered. Namely, only these irreps that actually appear in Eq. (1) are relevant, which substantially reduces the search space of candidate MSGs compared with a brute-force subgroup search, as shown in the Mn_3GaN example below.

In general, the magnetic structure is still not uniquely determined even after both the unstable irrep and its corresponding MSGs are fixed, except in the special case where $j = 1$ and $n_i = 1$. In this special case where Γ_{mag} contains only one-dimensional irreps ($j = 1$) and each irrep appears only once ($n_i = 1$), the basis vectors of irreps are uniquely fixed. As a result, the magnetic structure is uniquely determined since there is no other freedom of the selection of basis vectors.

However, Γ_{mag} generally contains multidimensional irreps ($j > 1$) and/or repeated occurrences ($n_i > 1$), as also demonstrated in the following benchmark section; in this situation, additional degrees of freedom remain within the irrep space. This leads to the non-uniqueness of the magnetic configuration, even after the relevant irrep and its compatible MSGs are fixed. A more proper strategy for constructing explicit magnetic configurations is therefore to employ the symmetry-adapted basis vectors of the irrep. Nevertheless, residual degrees of freedom may remain within this basis-vector description; in the following, we introduce two strategies to systematically constrain these freedoms and generate a finite set of predetermined magnetic structures.

Strategy I: multidimensional irreps ($j > 1$). For multi-dimensional irreducible representations $\Gamma_i(j)$ with $j > 1$ in Eq. (1), the set of the order parameter within the irrep space is not uniquely fixed, and different symmetry-allowed choices generally correspond to different MSGs. In principle, the physically realized order parameter could be determined by minimizing the higher-order terms of the Landau free energy. In the present work, however, we do not pursue such an explicit free-energy minimization. Instead, we adopt a symmetry-based criterion and retain **all** the maximal-symmetry magnetic subgroups among those compatible with the irrep in Eq. (1). Physically, ordering patterns belonging to these MSGs correspond to minimal symmetry breaking at the magnetic transition and therefore provide a natural representative set for screening [3, 4]. Consistent with this strategy, our benchmark shows that **100%** of the surveyed materials follow the maximal-symmetry selection rule, as shown in the Benchmark section.

Strategy II: repeated irreps ($n_i > 1$). A second source of non-uniqueness arises when a given irrep appears multiple times in the representation, i.e., $n_i > 1$ in Eq. (1). In this case, multiple symmetry-equivalent sets of the basis vectors exist and can be linearly combined with one another, leading to an infinite number of possible predetermined magnetic configurations. To systematically remove this redundancy and generate a finite set of configurations, we retain only those basis vectors that generate magnetic configurations with moments aligned along all possible high-symmetry crystallographic directions compatible with the corresponding MSGs. This strategy captures the majority of experimentally reported magnetic structures, as shown in the benchmark below.

Example: Mn_3GaN. We take Mn_3GaN as a representative example [5] to illustrate our workflow. Mn_3GaN belongs to the antiperovskite Mn_3AN family and has attracted considerable interest due to its noncollinear antiferromagnetism and its relevance to Hall-type transport responses, whose measured signals are highly sensitive to the underlying symmetry of the magnetic structure [6–9].

Mn_3GaN crystallizes in the cubic space group $Pm\bar{3}m$ (No. 221) [5]. This parent symmetry admits **98** distinct MSGs and **10** inequivalent irreducible representations (counting each irrep only once), all of which can, in principle, serve as symmetry-breaking channels for magnetic ordering. The **10** inequivalent irreducible representations of $Pm\bar{3}m$ are listed in Table S1.

Instead of considering all these **10** irreps in Table S1 which are admitted by the parent space group $Pm\bar{3}m$, we take the local magnetic-moment components $\boldsymbol{\mu}$ of Mn, which occupy the $3c$ Wyckoff positions, as the basis to construct the representation for Mn_3GaN. Since the unit cell contains three Mn atoms ($N = 3$), the magnetic degrees of freedom consist of $3N = 9$ magnetic-moment components,

$$\boldsymbol{\mu} = (m_{1x}, m_{1y}, m_{1z}, m_{2x}, m_{2y}, m_{2z}, m_{3x}, m_{3y}, m_{3z}), \tag{2}$$

which form a natural basis for the magnetic representation Γ_{mag} of the parent space group G. Here, the subscripts 1, 2, and 3 label the three Mn ions occupying the Wyckoff $3c$ positions at $(x, y, z) = (\frac{1}{2}, \frac{1}{2}, 0)$, $(\frac{1}{2}, 0, \frac{1}{2})$, and $(0, \frac{1}{2}, \frac{1}{2})$, respectively. Decomposing the representation Γ_{mag} into irreducible representations yields,

$$\Gamma_{\mathrm{mag}} = 2 \times \Gamma_4^+(3) \oplus 1 \times \Gamma_5^+(3), \tag{3}$$

where the superscript $+$ denotes even parity under inversion. Both $\Gamma_4^+(3)$ and $\Gamma_5^+(3)$ are three-dimensional ($j = 3$) irreps of the parent space group $Pm\bar{3}m$.

TABLE S1. Character table for the irreducible representations of the point group $m\bar{3}m$ (No. 32), corresponding to the Γ point of crystallographic space group No. 221 ($Pm\bar{3}m$)[10]. The point group contains ten conjugacy classes, denoted as $\boldsymbol{C_1}$-$\boldsymbol{C_{10}}$. The symmetry operations in $\boldsymbol{C_1}$-$\boldsymbol{C_{10}}$ are listed as follows:

$\boldsymbol{C_1}$: 1
$\boldsymbol{C_2}$: $2_{001}, 2_{010}, 2_{100}$
$\boldsymbol{C_3}$: $2_{01\bar{1}}, 2_{011}, 2_{1\bar{1}0}, 2_{\bar{1}01}, 2_{101}, 2_{110}$
$\boldsymbol{C_4}$: $3^-_{\bar{1}1\bar{1}}, 3^-_{1\bar{1}\bar{1}}, 3^+_{1\bar{1}\bar{1}}, 3^+_{\bar{1}\bar{1}1}, 3^+_{\bar{1}1\bar{1}}, 3^+_{111}, 3^-_{\bar{1}\bar{1}1}, 3^-_{\bar{1}\bar{1}\bar{1}}$
$\boldsymbol{C_5}$: $4^+_{001}, 4^-_{010}, 4^+_{010}, 4^-_{001}, 4^+_{100}, 4^-_{100}$
$\boldsymbol{C_6}$: $\bar{1}$
$\boldsymbol{C_7}$: $m_{001}, m_{010}, m_{100}$
$\boldsymbol{C_8}$: $m_{01\bar{1}}, m_{011}, m_{1\bar{1}0}, m_{\bar{1}01}, m_{101}, m_{110}$
$\boldsymbol{C_9}$: $\bar{3}^-_{\bar{1}1\bar{1}}, \bar{3}^-_{1\bar{1}\bar{1}}, \bar{3}^+_{1\bar{1}\bar{1}}, \bar{3}^+_{\bar{1}\bar{1}1}, \bar{3}^+_{\bar{1}1\bar{1}}, \bar{3}^+_{111}, \bar{3}^-_{\bar{1}\bar{1}1}, \bar{3}^-_{111}$
$\boldsymbol{C_{10}}$: $\bar{4}^+_{001}, \bar{4}^-_{010}, \bar{4}^+_{010}, \bar{4}^-_{001}, \bar{4}^+_{100}, \bar{4}^-_{100}$

	C_1	C_2	C_3	C_4	C_5	C_6	C_7	C_8	C_9	C_{10}
Γ_1^+	1	1	1	1	1	1	1	1	1	1
Γ_1^-	1	1	1	1	1	-1	-1	-1	-1	-1
Γ_2^+	1	1	-1	1	-1	1	1	-1	1	-1
Γ_2^-	1	1	-1	1	-1	-1	-1	1	-1	1
Γ_3^+	2	2	0	-1	0	2	2	0	-1	0
Γ_3^-	2	2	0	-1	0	-2	-2	0	1	0
Γ_4^+	3	-1	-1	0	1	3	-1	-1	0	1
Γ_4^-	3	-1	-1	0	1	-3	1	1	0	-1
Γ_5^+	3	-1	1	0	-1	3	-1	1	0	-1
Γ_5^-	3	-1	1	0	-1	-3	1	-1	0	1

It is evident from Eq. (3) that, incorporating the Mn atoms at the $3c$ Wyckoff positions reduces the set of irreps relevant for magnetic ordering of Mn_3GaN. Specifically, the original **10** irreps of the parent space group $Pm\bar{3}m$ are reduced to only **2** relevant irreps, Γ_4^+ and Γ_5^+. This irrep reduction immediately and substantially constrains the space of symmetry-allowed magnetic orderings.

As a consequence, instead of considering all **98** magnetic space groups compatible with $Pm\bar{3}m$, only the **9** magnetic space groups associated with Γ_4^+ and Γ_5^+ need to be examined, namely $R\bar{3}m'$, $R\bar{3}m$, $P4/mm'm'$, $P4'/mm'm$, $Cmm'm'$, $C2'/m'$, $C2/m$, $P2'/m'$, and $P\bar{1}$. This represents an effective reduction of the MSG search space by approximately one order of magnitude.

For Mn_3GaN, the representation $\Gamma_{\rm mag}$ contains two copies of $\Gamma_4^+(3)$ and one copy of $\Gamma_5^+(3)$, i.e., $n_4 = 2$ and $n_5 = 1$ in Eq. (3). Both irreducible representations are three-dimensional ($j = 3$). Mn_3GaN therefore provides a prototypical example in which both intrinsic sources of magnetic-structure non-uniqueness are present: (i) the freedom of the order parameter within a multidimensional irrep ($j > 1$), and (ii) the basis ambiguity associated with repeated irreps ($n_i > 1$).

We first address the ambiguity associated with multidimensional irreps by applying the maximal-symmetry criterion. This further reduces the **9** symmetry-compatible magnetic space groups to a compact set of **5** maximal magnetic subgroups (with duplicated MSGs counted only once). Specifically, the maximal-symmetry MSGs are $R\bar{3}m'$, $P4/mm'm'$, and $Cmm'm'$ for the Γ_4^+ channel, and $R\bar{3}m$, $P4'/mm'm$, and $Cmm'm'$ for the Γ_5^+ channel, as illustrated in Fig. (S1).

In Mn_3GaN, the irreducible representation Γ_4^+ appears twice in the magnetic representation, i.e., $n_4 = 2$, and its dimensionality $j = 3$. As a direct consequence, two independent but symmetry-equivalent sets of symmetry-adapted basis vectors are associated with Γ_4^+. These two basis sets, denoted as $\{\boldsymbol{\phi}_l^{(a)}\}$ with $a \in \{1, 2\}$ labeling the two symmetry-equivalent copies of Γ_4^+ and $l = 1, 2, 3$ labeling its dimensionality, are explicitly given by

$$\begin{aligned}
\boldsymbol{\phi}_1^{(1)} &= (1,0,0;\ 1,0,0;\ 0,0,0),\\
\boldsymbol{\phi}_2^{(1)} &= (0,1,0;\ 0,0,0;\ 0,1,0),\\
\boldsymbol{\phi}_3^{(1)} &= (0,0,0;\ 0,0,1;\ 0,0,1),
\end{aligned} \tag{4}$$

and

$$\begin{aligned}
\boldsymbol{\phi}_1^{(2)} &= (0,0,0;\ 0,0,0;\ 1,0,0),\\
\boldsymbol{\phi}_2^{(2)} &= (0,0,0;\ 0,1,0;\ 0,0,0),\\
\boldsymbol{\phi}_3^{(2)} &= (0,0,1;\ 0,0,0;\ 0,0,0).
\end{aligned} \tag{5}$$

We first apply the maximal-symmetry criterion (Strategy I) to identify the candidate magnetic space groups associated with Γ_4^+. As shown in Fig. S1, three maximal-symmetry MSGs are obtained, namely $R\bar{3}m'$, $P4/mm'm'$, and $Cmm'm'$. Taking the maximal magnetic subgroup $R\bar{3}m'$ (No. 166.101) as an example, the basis vectors of the Γ_4^+ irrep compatible with this MSG can be constructed as linear combinations of the irrep basis functions:

$$\boldsymbol{\eta}^{(1)} \propto \boldsymbol{\phi}_1^{(1)} + \boldsymbol{\phi}_2^{(1)} + \boldsymbol{\phi}_3^{(1)}, \qquad \boldsymbol{\eta}^{(2)} \propto \boldsymbol{\phi}_1^{(2)} + \boldsymbol{\phi}_2^{(2)} + \boldsymbol{\phi}_3^{(2)}. \tag{6}$$

In general, for the maximal MSG $R\bar{3}m'$ (No. 166.101), the basis vectors can be expressed as linear superpositions of these two basis sets,

$$\boldsymbol{\eta} = \alpha\,\boldsymbol{\eta}^{(1)} + \beta\,\boldsymbol{\eta}^{(2)}, \tag{7}$$

where real numbers α and β are free parameters, which reflects the intrinsic basis ambiguity associated with repeated irreducible representations ($n_i > 1$).

For a given choice of (α, β), based on Eqs. (4)-(14), the resulting magnetic moments on the three Mn ions of Mn_3GaN can be written as:

$$\boldsymbol{\mu} \propto (\alpha, \alpha, \beta;\ \alpha, \beta, \alpha; \beta, \alpha, \alpha), \tag{8}$$

which illustrates that infinite magnetic configurations are symmetry-allowed at this stage.

Then, to construct a finite and physically relevant set of magnetic structures, we impose an additional constraint by retaining only those basis vectors that generate magnetic moments aligned along high-symmetry crystallographic directions. For Mn_3GaN with space group $Pm\bar{3}m$, these typically directions include the fourfold ([100], [010], [001]), threefold ([111], [$1\bar{1}1$], [$\bar{1}11$], [$11\bar{1}$]), and twofold ([$1\bar{1}0$], [110], [$01\bar{1}$], [011], [$\bar{1}01$], [101]) rotational axes, as well as in-plane directions perpendicular to the threefold axes ([112], [$\bar{1}12$], [$1\bar{1}2$], [$\bar{1}\bar{1}2$], [121], [$\bar{1}21$], [$12\bar{1}$], [$\bar{1}2\bar{1}$], [211], [$2\bar{1}1$], [$21\bar{1}$], [$2\bar{1}\bar{1}$]) [11].

For MSG $R\bar{3}m'$ (No. 166.101) of Mn_3GaN, we take the Mn ion at $(\frac{1}{2}, \frac{1}{2}, 0)$ as a representative site (the magnetic moments on the other two Mn ions are then fixed by applying the C_3 symmetry operation), the corresponding local magnetic moment is given by

$$(m_{1x},\, m_{1y},\, m_{1z}) \propto (\alpha,\, \alpha,\, \beta), \tag{9}$$

which corresponds to the first three components of Eq. (8). By comparing this direction with the aforementioned 25 high-symmetry crystallographic directions of the space group $Pm\bar{3}m$, only 6 distinct possibilities are allowed. These correspond to the following high-symmetry directions:

$$\begin{array}{lll} [001]\ (\alpha=0,\beta=1), & [111]\ (\alpha=\beta=1), & [\bar{1}\bar{1}1]\ (\alpha=-1,\beta=1), \\ [110]\ (\alpha=1,\beta=0), & [112]\ (\alpha=1,\beta=2), & [\bar{1}\bar{1}2]\ (\alpha=-1,\beta=2), \end{array} \tag{10}$$

as summarized (a)-(f) panels in Table S2. Since these configurations correspond to the maximal MSG $R\bar{3}m'$ (No. 166.101) associated with the irrep Γ_4^+, it can be constructed straightforwardly following the procedure in Eqs. (6)–(10). In particular, the magnetic moment of the Mn ion at $(\frac{1}{2}, \frac{1}{2}, 0)$ is constrained to and only to the six high-symmetry directions listed in Eq. (10). As an illustrative example, the configuration shown in panel (a) of Table S2 corresponds to choosing $\alpha = 0$ and $\beta = 1$ in Eq. (10), yielding the magnetic moment of Mn ion at $(\frac{1}{2}, \frac{1}{2}, 0)$ aligned along the $[001]$ direction.

By repeating this procedure for all subgroups in Fig. (S1), we obtain a total of 11 predetermined magnetic configurations for Mn_3GaN, see Table S2 (including 7 noncollinear and 4 collinear magnetic configurations).

Although our irreducible-representation basis-vector strategy considers only 11 initial magnetic configurations, notably, the experimentally reported magnetic structure as in **panel (k)** of Table S2 is already included in this candidate set; this structure belongs to the Γ_5^+ irrep and corresponds to MSG $R\bar{3}m$ (No. 166.97).

More generally, as demonstrated in the Benchmark section below, the majority of experimental magnetic structure in the MAGNDATA database are captured by our irrep basis-vector strategy. Consequently, with sufficiently accurate total-energy calculations, the correct magnetic structure can be identified by energy ranking within these compact candidate sets.

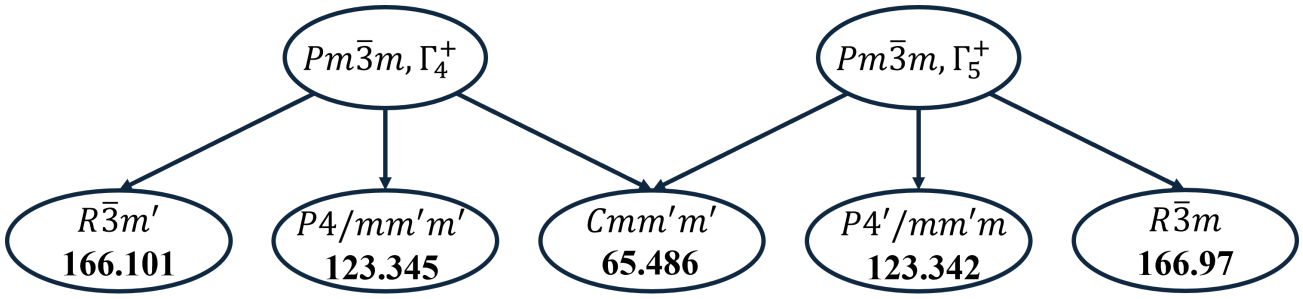


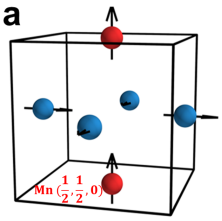
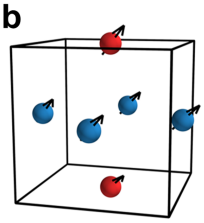
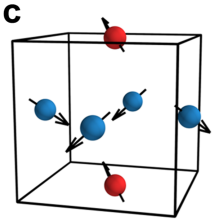
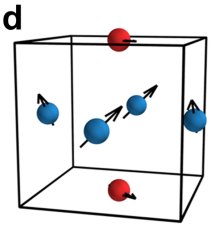
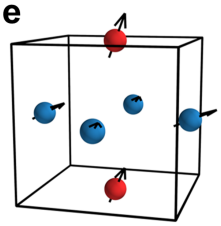
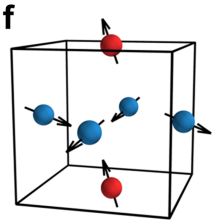
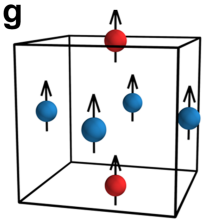
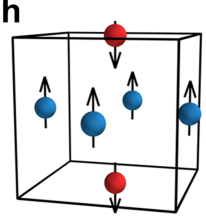
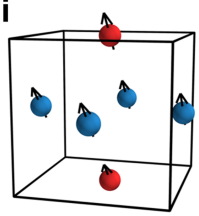
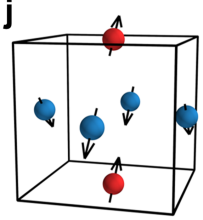
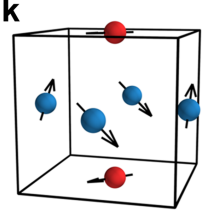
FIG. S1. **Symmetry-compatible MSGs for Mn_3GaN.** Maximal-symmetry candidate MSGs associated with the irreducible representations Γ_4^+ and Γ_5^+.

B. First-principles Total-Energy Screening for the Magnetic Structure

Based on the finite number of initial states selected by our irrep basis-vector strategy, first-principles total-energy calculations were then performed among these well-selected structures using the Vienna Ab initio Simulation Package (VASP) [12, 13], employing a spin-polarized GGA + SOC + U approach. The Coulomb interaction parameters U and Hund J were taken as the averaged values recommended for transition-metal elements based on the linear-response scheme [14]. The k-mesh of the Brillouinzone is set by $60/a$ along each direction, where a denotes the length of the lattice constant in Å.

For Mn_3GaN, U and J were set to $U = 4.8$ eV and $J = 0.7$ eV. A $17 \times 17 \times 17$ k-point mesh was employed for the first-principles calculations. By comparing the total energies of the 11 candidate magnetic configurations listed in Table S2, we identify the magnetic structure of Mn_3GaN as the one shown in **panel (k)**, which belongs to the $\Gamma_5^+(3)$ irrep in Eq. (3) and corresponds to the MSG $R\bar{3}m$ (No. 166.97), consistent with the experimentally reported ground state [5].

TABLE S2. Candidate magnetic structures for Mn_3GaN, generated using our irreducible-representation basis-vector strategy. For each configuration, we list the magnetic structure, the associated irreducible representation, MSG and the magnetic moment direction of the Mn atom at $(\frac{1}{2}, \frac{1}{2}, 0)$, which is chosen as a representative site to visualize the noncollinear nature of different magnetic configurations.

Magnetic Configration	a 	b 	c 	d 
Irreducible Representations	Γ_4^+	Γ_4^+	Γ_4^+	Γ_4^+
MSG	$R\bar{3}m'$ (166.101)	$R\bar{3}m'$ (166.101)	$R\bar{3}m'$ (166.101)	$R\bar{3}m'$ (166.101)
Moment Direction of Mn (1/2, 1/2, 0)	[001]	[111]	$[\bar{1}\bar{1}1]$	[110]
Magnetic Configration	e 	f 	g 	h 
Irreducible Representations	Γ_4^+	Γ_4^+	Γ_4^+	Γ_4^+
MSG	$R\bar{3}m'$ (166.101)	$R\bar{3}m'$ (166.101)	$P4/mm'm'$ (123.345)	$P4/mm'm'$ (123.345)
Moment Direction of Mn (1/2, 1/2, 0)	[112]	$[\bar{1}\bar{1}2]$	[001]	$[00\bar{1}]$
Magnetic Configration	i 	j 	k 	
Irreducible Representations	Γ_4^+	Γ_4^+	Γ_5^+	
MSG	$Cmm'm'$(65.486)	$Cmm'm'$(65.486)	$R\bar{3}m$ (166.97)	
Moment Direction of Mn (1/2, 1/2, 0)	[101]	$[\bar{1}01]$	$[1\bar{1}0]$	

C. Irreducible-Representation Basis-Vector Construction of Initial Magnetic Structures for $q \neq 0$ using CrSBr as an example

For the case of $q \neq 0$, we take CrSBr as an illustrative example. CrSBr crystallizes in the space group $Pmmn$ (No. 59) [15]. Its magnetic structure can be described as a spin-density-wave modulation of the paramagnetic phase, characterized by a single independent propagation vector $\mathbf{q} = (0, 0, 1/2)$, as determined experimentally from diffraction measurements [15].

For the propagation vector $\mathbf{q} = (0, 0, 1/2)$, the little group $G_{\mathbf{q}}$ contains eight symmetry operations, and correspondingly admits eight inequivalent irreducible representations (counting each irrep only once). The character table of these eight irreducible representations, denoted as $Z_i^{\pm}$ $(i = 1, \ldots, 4)$, is listed in Table S3.

TABLE S3. Character table for the irreducible representations at the $\mathbf{q} = (0, 0, 1/2)$ point of crystallographic space group No. 59 ($Pmmn$) [10]. The little group $G_{\mathbf{q}}$ contains 8 symmetry operation, denoted as $\boldsymbol{C_1}$-$\boldsymbol{C_8}$, which are listed as follows:

$\boldsymbol{C_1}$: 1 $\boldsymbol{C_2}$: $\{2_{001}|1/2, 1/2, 0\}$ $\boldsymbol{C_3}$: $\{2_{010}|0, 1/2, 0\}$ $\boldsymbol{C_4}$: $\{2_{100}|1/2, 0, 0\}$
$\boldsymbol{C_5}$: $\bar{1}$ $\boldsymbol{C_6}$: $\{m_{001}|1/2, 1/2, 0\}$ $\boldsymbol{C_7}$: $\{m_{010}|0, 1/2, 0\}$ $\boldsymbol{C_8}$: $\{m_{100}|1/2, 0, 0\}$

	C_1	C_2	C_3	C_4	C_5	C_6	C_7	C_8
Z_1^+	1	1	1	1	1	1	1	1
Z_1^-	1	1	1	1	-1	-1	-1	-1
Z_2^+	1	1	-1	-1	1	1	-1	-1
Z_2^-	1	1	-1	-1	-1	-1	1	1
Z_3^+	1	-1	-1	1	1	-1	-1	1
Z_3^-	1	-1	-1	1	-1	1	1	-1
Z_4^+	1	-1	1	-1	1	-1	1	-1
Z_4^-	1	-1	1	-1	-1	1	-1	1

In CrSBr, there are two Cr atoms occupy the $2b$ Wyckoff positions, labeling as 1 and 2 separately. The magnetic configuration can therefore be expressed in terms of the local magnetic-moment components of these two Cr atoms:

$$\boldsymbol{\mu} = (m_{1x}, m_{1y}, m_{1z}, m_{2x}, m_{2y}, m_{2z})\, e^{i2\pi\mathbf{q}\cdot\mathbf{R}}, \tag{11}$$

here $\mathbf{R}$ denotes the Bravais lattice vector labeling different unit cells along the propagation direction. For the propagation vector $\mathbf{q} = (0, 0, 1/2)$, $\mathbf{q} \cdot \mathbf{R} = 1/2,\ 1, \ldots$, namely $e^{i2\pi\mathbf{q}\cdot\mathbf{R}} = -1, 1, \ldots$ in Eq. (11), for successive unit cells along the c axis, corresponding to the phase modulation of the magnetic moments without explicitly constructing a real-space supercell.

By applying the symmetry operations of the little group $G_{\mathbf{q}}$ to the basis $\boldsymbol{\mu}$ in Eq. (11), we obtain a reducible magnetic representation Γ_{mag} at $\mathbf{q} = (0, 0, 1/2)$ of the parent space group G, as in Eq. (1). Decomposing this representation into irreducible components yields:

$$\Gamma_{\mathrm{mag}} = Z_1^-(1) \oplus Z_2^+(1) \oplus Z_3^+(1) \oplus Z_3^-(1) \oplus Z_4^+(1) \oplus Z_4^-(1), \tag{12}$$

The irreducible components yielded by the decomposition of Γ_{mag} correspond to the special case discussed above, namely the dimensionality of all irreps $j = 1$, and all irreps exist once corresponding $n_i = 1$.

As discussed in the main text and in Section I. A of the Supplemental Materials, in this special case where all decomposed irreps satisfy $n_i = 1$ and each irrep admits a single basis function ($j = 1$), the symmetry-adapted basis vectors are uniquely fixed and fully determine the magnetic structure.

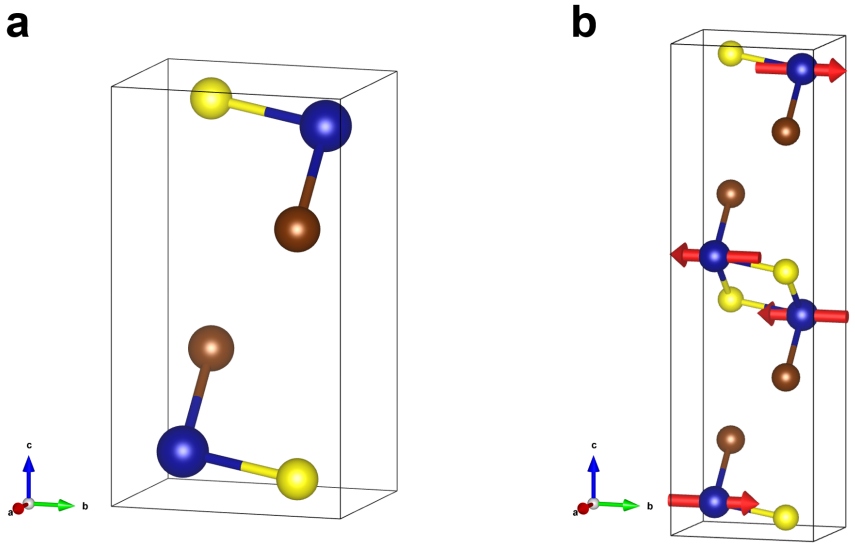


FIG. S2. (a) Crystal structure of CrSBr with Cr atoms shown in blue, S atoms in yellow, and Br atoms in brown. (b) Experimentally reported magnetic structure of CrSBr [15].

The irreducible representation Z_4^+, which corresponds to the experimentally reported magnetic ground state of CrSBr [15], has already been captured by Eq. (12). To obtain the corresponding magnetic basis vector, we apply the projection operator of Z_4^+ to the basis $\boldsymbol{\mu}$ in

Eq. (11). This uniquely procedure yields the irrep basis function:

$$\boldsymbol{\phi}_1 = (0, -1, 0;\ 0, 1, 0), \tag{13}$$

and then the basis vectors can be expressed as:

$$\boldsymbol{\eta} \propto (0, -1, 0;\ 0, 1, 0)\ e^{i2\pi\mathbf{q}\cdot\mathbf{R}}\ , \tag{14}$$

the corresponding magnetic structure is illustrated in Fig. S2 (b).

D. Comparison with Recent Spin-Symmetry-Adapted Approaches for Magnetic Structure Prediction

Spin space group (SSG) was first introduced in 1960s [16, 17] to describe the magnon band feature neglecting the Dzyaloshinskii-Moriya interaction (DMI), which is the leading order of spin-orbit coupling (SOC) effect [18–20]. In recent years, SSG has been extended to electronic systems with negligible SOC [21] and has attracted increasing attention as a powerful tool for analyzing the spintronics [22], band structures [23, 24], topology [25, 26], transport phenomena [27, 28] *etc*.

Very recently, two independent studies have employed SSGs and oriented SSGs frameworks [29], in combination with first-principles calculations, to determine magnetic structures [30, 31]. In the following, we briefly summarize these approaches and compare them with our method.

Nomoto *et al.* developed a symmetry-guided framework for magnetic structures prediction based on spin-symmetry-adapted (SSA) structures [31]. In their approach, magnetic structures are constructed in the form of SSA structures, which are obtained using projection operators to enforce the symmetry constraints of a given SSG. These SSA structures represent exchange-dominated magnetic structures that are invariant under the corresponding SSG operations [31].

To consider SOC effects, the authors further employ the concept of oriented SSA structures [29]. By applying global spin rotations and selecting orientations that induce maximal MSGs, SSA structures are mapped onto a finite set of crystallographically distinct configurations. This procedure enables a systematic enumeration of candidate magnetic structures. As noted in their work, this method is not applicable to materials with magnetic atoms occupied multiple inequivalent Wyckoff positions [31].

To assess the performance of their framework, Nomoto *et al.* benchmarked their method against a dataset of experimentally reported magnetic structures. The overall procedure consists of two main steps. In the first step, SSA structures are generated for all candidate materials collected from the MAGNDATA database [32], from which 1023 experimentally reported magnetic compounds are selected for subsequent analysis. Among them, SSGs of magnetic structures of 623 cases are fully reproduced and SSGs of magnetic structures of 168 cases are partially reproduced at the SSA level, in the sense that the dominant features of the experimentally reported magnetic structures are correctly captured. This corresponds to an overall reproduction rate of $(623 + 168)/1023 \approx 77.3\%$ [31].

Based on the SSA structures mentioned above, oriented SSA structures are constructed for SOC refinement. Among the SSGs of magnetic structures of 623 fully reproduced SSA cases, 511 materials are further reproduced at the oriented-SSA level, corresponding to a success rate of approximately $511/623 \approx 82.0\%$ at this step [31].

Secondly, the symmetry-generated magnetic candidates are further filtered and selected by first-principles calculations in two stages. First, they perform self-consistent (SCF) first-principles calculations without SOC to evaluate the total energies of the SSA structures and identify the lowest-energy magnetic geometry [31]. Then, to incorporate SOC effects on magnetic orientations, they carry out non-self-consistent calculations with SOC, in which the charge density is fixed to that obtained from the SOC-free SCF step, and the energies of the corresponding oriented-SSA descendants are compared to determine the preferred orientation [31]. This strategy is designed to exploit the separation of energy scales between exchange interactions and SOC-induced anisotropy, and is typically used in situations where SOC is expected to induce only a very small change in the self-consistent charge density.

In parallel, Li *et al.* proposed a symmetry-based workflow for magnetic-structure prediction based on SSGs [30]. They distinguish between exchange-dominated *magnetic geometries* (relative spin arrangements) and SOC-selected *magnetic configurations* (geometries with constrained orientations). In their framework, candidate geometries are generated by enumerating space-group subgroups G_0 of the parent structure and constructing the corresponding SSG-allowed spin arrangements using an SSG Wyckoff-position database [30].

To incorporate SOC effects, constrained spin orientations are enumerated for the magnetic geometry using the corresponding MSGs. These MSG-derived orientations define a finite set of symmetry-allowed magnetic configurations, whose relative energies are subsequently evaluated by first-principles calculations. In this way, SOC-induced anisotropy is taken into account through energetic selection within the geometry class [30].

Similar to the approach of Nomoto *et al.* [31], the workflow of Li *et al.* also consists of two main stages and follows a closely related computational procedure. First, SOC-free structure first-principless calculations are performed to identify low-energy magnetic geometries. Second, SOC is included in subsequent calculations to determine the preferred magnetic configuration. To control the size of the search space, practical constraints limiting the magnetic cell expansion factor (no more than fourfold) and restricting the set of considered space-group subgroups are employed. Using this procedure, Li *et al.* validated their framework on several representative unconventional magnets, including MnTe, Mn_3Sn, and $CoNb_3S_6$, and reported that their first-principles results are in agreement with the experimentally observed magnetic structures for these cases [30].

Different from SSG-based approaches, our strategy is rooted in Landau theory and is formulated in terms of MSGs and basis vectors of irreps, our method naturally bypasses the need to treat spin–orbit coupling as a separate perturbation. At the same time, multiple inequivalent Wyckoff positions are treated on an equal footing, avoiding the intrinsic restrictions encountered in single-Wyckoff-positions schemes. This strategy can therefore be applied uniformly across materials with either weak or sizeable SOC, within the same computational protocol. More importantly, the physically grounded nature of our approach enables the efficient and reliable construction of large-scale magnetic structure databases.

II. DETAILS OF BENCHMARK TESTING USING THE MAGNDATA DATABASE

The discrepancies between the magnetic structure obtained from our irrep basis-vector strategy and the experimentally reported magnetic structures originate from two distinct factors: (1) the experimental magnetic structure is not included in the set of our initial candidate magnetic configurations. This limitation is intrinsic to our irrep basis-vector strategy, arising from our "all possible high-symmetry crystallographic directions compatible with the corresponding irrep" strategy used to address the presence of repeated irreducible representations (i.e., $n_i > 1$ in Eq. (1)); (2) the experimental magnetic structure is included in the initial input set, but first-principles total-energy calculations fail to identify it as the lowest-energy state. The latter issue is, in principle, addressable through enhanced computational resources and more efficient algorithms.

In the following, we benchmark these two aspects separately by systematically examining experimentally established magnetic structures documented in the MAGNDATA database [32].

A. Accuracy of Our Strategy for Selecting Input Magnetic Structures

We restrict our analysis to stoichiometric materials with fewer than 40 atoms per unit cell and a zero propagation vector ($\mathbf{q} = 0$). Only materials that explicitly contain transition-metal ions are considered, while lanthanoid and actinoid ions are excluded due to the challenges in accurately described within standard density functional theory [33]. These criteria reduce the MAGNDATA dataset to 328 materials, which serve as benchmark cases for evaluating our irrep basis-vector strategy.

Among these 328 materials, 26 entries do not satisfy the criteria for continuous magnetic phase transitions considered in this work, as they cannot be characterized by a single irreducible representation of the crystallographic space group, which possibly due to the structural phase transitions, magnetoelastic coupling, etc. Detailed information on these 26 magnetic materials is provided in Table S4. The remaining 302 materials therefore fall within the applicability range of our irrep basis-vector strategy.

We first analyze the magnetic structure of these 302 materials as reported in MAGNDATA. Among them, the experimental magnetic structure of 76 materials correspond to a one-dimensional irreducible representation appearing only once, i.e., the case with $j = 1$ and $n_i = 1$ in Eq. (1), as listed in Table S5. In this situation, the associated basis vectors of this irrep are uniquely fixed by symmetry, and consequently, the magnetic structure is uniquely determined without additional constraints. These cases therefore admit no any ambiguity and are fully captured by our framework by construction, namely, the magnetic structures of these materials are included in our initial magnetic configuration set.

We now turn to examine the ambiguity associated with multidimensional irreducible representations (i.e., cases with $n_i = 1$ and $j > 1$ in Eq. (1)). For such cases, the order parameter within the irrep space is not uniquely determined, corresponding to different MSGs, giving rise to an intrinsic ambiguity in the magnetic configurations. Among the remaining 226 materials in our benchmark set, 12 fall into this category, as summarized in Table S6. To resolve this ambiguity, our irrep basis-vector strategy adopts a maximal-symmetry criterion: instead of attempting to determine the order-parameter direction by explicitly minimizing higher-order Landau free-energy terms, we retain the magnetic structures associated with maximal symmetry magnetic subgroups compatible with the given multidimensional irrep. Remarkably, without exception, the experimentally reported magnetic structure of all 12 materials are consistent with this maximal magnetic subgroup scenario. This benchmark therefore demonstrates that the maximal-symmetry criterion resolves the ambiguity associated with multidimensional irreducible representations ($j > 1$) with **100% success** for all materials examined — meaning the corresponding magnetic structures are also successfully contained within our set of initial magnetic configurations.

We then turn to the ambiguity arising from repeated irreducible representations ($n_i > 1$). Among the remaining 214 materials, magnetic moments deviate from high-symmetry directions in 49 materials, which fall outside the scope of our irrep basis-vector strategy, as summarized in Table S7. The remaining 165 cases exhibit magnetic moments aligned along high-symmetry directions and are therefore successfully captured by our irrep basis-vector strategy, as listed in Table S8.

Consequently, for 253 out of the 302 benchmark materials (83.8%), the experimentally reported magnetic structure fall within the very limited ($\sim$20) candidate set generated by our irrep basis-vector strategy.

TABLE S4. A detailed list of 26 magnetic structures incompatible with a continuous phase transition is provided, including the MAGNDATA labels, chemical formulas, crystallographic space groups, magnetic space groups, and irreducible representations of the crystallographic space group. Material names are followed by their corresponding labels (in parentheses) from the MAGNDATA database [32].

Materials	Crystallographic space group	Magnetic space group	Irreps
Fe_4O_5 (0.999) [34]	$Cmcm$ (No.63)	$Cm'c2'_1$ (No.36.174)	Γ_3^-, Γ_4^+
Fe_4O_5 (0.1000) [34]	$Cmcm$ (No.63)	$P2'_1$ (No.4.9)	$\Gamma_3^-, \Gamma_4^+, \Gamma_3^+$
$BaFe_2Se_4$ (0.1024)[35]	$I4/m$ (No.87)	$C2'$ (No.5.15)	$\Gamma_3^+\Gamma_4^+, \Gamma_3^-\Gamma_4^-$
$Mn_3Si_2Te_6$ (0.1026)[36]	$P\bar{3}1c$ (No.163)	$C2'/c'$ (No.15.89)	Γ_3^+, Γ_2^+
$LuFe_4Ge_2$ (0.140)[37]	$P4_2/mnm$ (No.136)	$Pn'n'm'$ (No.58.399)	Γ_2^-, Γ_2^+
$LiFePO_4$ (0.152)[38]	$Pnma$ (No.62)	$P2_1/c'$ (No.14.78)	Γ_2^-, Γ_1^-
$CaMnGe_2O_6$ (0.155) [39]	$C2/c$ (No.15)	$P\bar{1}'$ (No.2.6)	Γ_2^-, Γ_1^-
$SrMn(VO_4)(OH)$ (0.165)[40]	$P2_12_12_1$ (No.19)	$P2_1$ (No.4.7)	Γ_1, Γ_3
$FePO_4$ (0.17) [41]	$Pnma$ (No.62)	$P2_12_12_1$ (No.19.25)	Γ_1^-, Γ_1^+
$Co_4Nb_2O_9$ (0.196) [42]	$P\bar{3}c1$ (No.165)	$C2/c'$ (No.15.88)	Γ_3^-, Γ_1^-
Mn_3Ge (0.203)[43]	$P6_3/mmc$ (No.194)	$C2'/m'$ (No.12.62)	Γ_6^+, Γ_2^+
$RbMnF_4$ (0.329)[44]	$P2_1/a$ (No.14)	$P\bar{1}$ (No.2.4)	Γ_1^+, Γ_2^+
$LiCoPO_4$ (0.384)[45]	$Pnma$ (No.62)	$P2'_1/c$ (No.14.77)	Γ_2^-, Γ_4^-
$LiCoPO_4$ (0.385)[46]	$Pnma$ (No.62)	$P2_1/c'$ (No.14.78)	Γ_2^-, Γ_1^-
$YMnO_3$ (0.44)[47]	$P6_3cm$ (No.185)	$P6'_3$ (No.173.131)	Γ_3, Γ_4
La_2NiO_4 (0.45)[48]	$P4_2/ncm$ (No.138)	$Pc'c'n$ (No.56.369)	Γ_3^+, Γ_4^+
Cr_2S_3 (0.5)[49]	$R\bar{3}$ (No.148)	$P\bar{1}$ (No.2.4)	$\Gamma_2^+\Gamma_3^+, \Gamma_1^+$
$NaCrSi_2O_6$ (0.504)[50]	$C2/c$ (No.15)	$P\bar{1}'$ (No.2.6)	Γ_1^-, Γ_2^-
$CaMn_2Sb_2$ (0.523)[51]	$P\bar{3}m1$ (No.164)	$P\bar{1}'$ (No.2.6)	Γ_3^-, Γ_1^-
CaMnGe (0.601)[52]	$P4/nmm$ (No.129)	$P2_1/m'$ (No.11.53)	Γ_2^-, Γ_5^-
CaMnGe (0.602)[52]	$P4/nmm$ (No.129)	$P2_1/m'$ (No.11.53)	Γ_2^-, Γ_5^-
Mn_3Ga (0.641)[53]	$I4/mmm$ (No.139)	$C2'/m'$ (No.12.62)	Γ_3^+, Γ_5^+
YVO_3 (0.788)[54]	$P2_1/b11$ (No.14)	$P\bar{1}$ (No.2.4)	Γ_1^+, Γ_2^+
NbMnP (0.803) [55]	$Pnma$ (No.62)	$Pm'n2'_1$ (No.31.125)	Γ_3^+, Γ_4^-
Fe_2WO_6 (0.812) [56]	$Pbcn$ (No.60)	$Pn'c2'$ (No.30.113)	Γ_3^+, Γ_2^-
$FeSb_2O_4$ (0.97) [57]	$P4_2/mbc$ (No.135)	$Pmc2_1$ (No.26.66)	Γ_2^+, Γ_5^-

TABLE S5. Table of 76 materials with experimental magnetic structure corresponding to a one-dimensional irreducible representation appearing only once [j=1, n_i=1 in Eq. (1)]. Material names are followed by their corresponding labels (in parentheses) from the MAGNDATA database [32].

Materials			
$AlFe_2B_2$ (0.414)	$Ba_2Mn_3Sb_2O_2$ (0.471)	$Ba_2MnSi_2O_7$ (0.229)	$BaCr_2As_2$ (0.365)
$BaMn_2As_2$ (0.18)	$BaMn_2Bi_2$ (0.89)	$BaMn_2Ge_2$ (0.605)	$BaMn_2Ge_2$ (0.606)
$BaMn_2P_2$ (0.464)	$BaMn_2Sb_2$ (0.470)	$BaMnSb_2$ (0.611)	Bi_2CuO_4 (0.348)
Bi_2CuO_4 (0.694)	$CaMn_2Ge_2$ (0.603)	$CaMn_2Ge_2$ (0.604)	$CaMnBi_2$ (0.72)
CaMnSi (0.599)	CaMnSi (0.600)	CoF_2 (0.178)	CoF_3 (0.334)
$CoTa_4Se_8$ (0.1036)	Cr_2O_3 (0.59)	$CrNb_4S_8$ (0.708)	CrSb (0.528)
Fe_2TeO_6 (0.142)	Fe_2TeO_6 (0.960)	$FeCO_3$ (0.116)	$KFeSe_2$ (0.637)
KMnBi (0.618)	$KMnF_3$ (0.433)	KMnSb (0.617)	$KOsO_4$ (0.284)
$KRuO_4$ (0.285)	$La_2O_3Mn_2Se_2$ (0.1091)	$La_2O_3Mn_2Se_2$ (0.1092)	$La_2O_3Mn_2Se_2$ (0.1093)
$LaBaMn_2O_6$ (0.737)	$LaBaMn_2O_6$ (0.738)	$LaCrO_3$ (0.416)	$LaMn_2Si_2$ (0.472)
$LaMn_2Si_2$ (0.498)	LaMnAsO (0.619)	LaMnAsO (0.624)	LaMnSbO (0.667)
$LaMnSi_2$ (0.778)	$LaMnSi_2$ (0.779)	$LaMnSi_2$ (0.780)	$LiCoPO_4$ (0.193)
$LiCoPO_4$ (0.383)	$LiFe_2F_6$ (0.501)	$LiFePO_4$ (0.95)	$MgMnO_3$ (0.277)
MnF_2 (0.15)	$MnGeO_3$ (0.125)	$MnTe_2$ (0.20)	NaMnAs (0.629)
NaMnAs (0.630)	NaMnBi (0.634)	NaMnBi (0.635)	NaMnP (0.626)
NaMnP (0.627)	NaMnP (0.628)	NaMnSb (0.631)	NaMnSb (0.632)
$NiCrO_4$ (0.896)	NiS_2 (0.150)	$PbNiO_3$ (0.21)	$RbFeSe_2$ (0.638)
RuO_2 (0.607)	$Sr_2Mn_3As_2O_2$ (0.212)	$Sr_4Fe_4O_{11}$ (0.401)	$SrCr_2As_2$ (0.364)
$SrMnBi_2$ (0.73)	$SrMnSb_2$ (0.767)	$YMnO_3$ (0.6)	$[Na(OH)_2]_3Mn(NCS)_3$ (0.1078)

TABLE S6. Table of 12 materials with multidimensional irreducible representations appearing only once [$n_i = 1$ and $j > 1$ in Eq. (1)]. All of their experimental magnetic structures fall in the scope of our irrep basis-vector strategy. Material names are followed by their corresponding labels (in parentheses) from the MAGNDATA database [32].

Materials			
$CaMn_2Sb_2$ (0.92)	Mn_2Au (0.1081)	Mn_2Au (0.639)	Mn_2Au (0.640)
Mn_3GaN (0.177)	Mn_3ZnN (0.273)	$MnNb_4S_8$ (0.709)	MnPtGa (0.395)
$MnTa_4S_8$ (0.711)	MnTe (0.800)	$SrMn_2As_2$ (0.482)	VNb_3S_6 (0.712)

TABLE S7. Table of 49 materials cannot be described by our method due to deviations of magnetic moments from high-symmetry directions, correspondng to the case when irreducible representations appeared multiple times [$n_i > 1$ in Eq. (1)] . Material names are followed by their corresponding labels (in parentheses) from the MAGNDATA database [32].

Materials				
Ag_2RuO_4 (0.918)	$BaFe_2Se_2O$ (0.988)	$BaMnFeF_7$ (0.577)	Ca_2MnReO_6 (0.204)	Ca_2RuO_4 (0.398)
$CaFe_5O_7$ (0.357)	Co_2SiO_4 (0.218)	Co_2SiO_4 (0.219)	$Co_4Nb_2O_9$ (0.197)	$Co_4Nb_2O_9$ (0.529)
$Co_4Ta_2O_9$ (0.511)	$CoFePO_5$ (0.262)	$CoSO_4$ (0.571)	$CoSO_4$ (0.96)	$CoSe_2O_5$ (0.119)
Cr_2F_5 (0.576)	$Cs_2Cu_3SnF_{12}$ (0.506)	$CsMn_2F_6$ (0.726)	$Cu_2(OD)_3Cl$ (0.295)	Cu_2OSO_4 (0.612)
$Fe(N(CN_2))_2$ (0.132)	Fe_2SeO (0.1061)	Fe_2SiO_4 (0.1072)	Fe_2SiO_4 (0.221)	Fe_2WO_6 (0.809)
Fe_2WO_6 (0.810)	GaV_4S_8 (0.756)	$KMnF_4$ (0.328)	La_2CoIrO_6 (0.375)	$LiNiPO_4$ (0.88)
Mn_2GeO_4 (0.101)	Mn_2GeO_4 (0.102)	Mn_2SiO_4 (0.220)	Mn_3CoGe (0.900)	Mn_3IrGe (0.899)
Mn_3IrSi (0.898)	Mn_3RhGe (0.1005)	Mn_3Sn_2 (0.663)	$MnNb_2O_6$ (0.819)	MnPtGa (0.396)
$MnTa_2O_6$ (0.818)	MnV_2O_4 (0.64)	$RbRuO_4$ (0.924)	$SrCo(VO_4)(OH)$ (0.287)	$SrFe_2S_2O$ (0.762)
$SrFe_2Se_2O$ (0.761)	Y_2MnCoO_6 (0.164)	YFe_4Ge_2 (0.27)	$ZrCo_2Ge_4O_{12}$ (0.314)	

TABLE S8. Table of 165 materials with experimental magnetic moments aligned along high-symmetry directions and compatible with our irrep basis-vector strategy, in the presence of repeated irreducible representations [$n_i > 1$, in Eq. (1)]. Material names are followed by their corresponding labels (in parentheses) from the MAGNDATA database [32].

Materials				
$Ba_2CoGe_2O_7$ (0.56)	$Ba_3NiRu_2O_9$ (0.748)	$BaCrF_5$ (0.303)	$BaCuF_4$ (0.191)	$BaFe_2S_2O$ (0.987)
$BaNi_2P_2O_8$ (0.215)	Bi_2CuO_4 (0.695)	$BiCrO_3$ (0.138)	$Ca_2Fe_2O_5$ (0.1080)	Ca_2FeOsO_6 (0.682)
Ca_2MnGaO_5 (0.825)	Ca_2NiOsO_6 (0.796)	$CaCu_3Fe_2Sb_2O_{12}$ (0.672)	$CaFe_2O_4$ (0.968)	$CaFe_2O_4$ (0.969)
$CaFe_4Al_8$ (0.236)	$CaFe_5O_7$ (0.358)	$CaIrO_3$ (0.79)	$CaMnGe_2O_6$ (0.156)	$Co_2Mo_3O_8$ (0.332)
$Co_2Mo_3O_8$ (0.338)	$Co_3Sn_2S_2$ (0.860)	$Co_3Sn_2S_2$ (0.861)	$Co_4Nb_2O_9$ (0.111)	$CoCO_3$ (0.114)
$CoSe_2O_5$ (0.161)	Cr_2CoAl (0.1073)	Cr_2MoO_6 (0.1023)	Cr_2O_3 (0.110)	Cr_2TeO_6 (0.143)
Cr_2TeO_6 (0.76)	Cr_2TeO_6 (0.959)	Cr_2WO_6 (0.144)	Cr_2WO_6 (0.75)	$CrSbSe_3$ (0.834)
$CsMnF_4$ (0.327)	$CuFePO_5$ (0.260)	$CuFeS_2$ (0.802)	CuMnAs (0.222)	CuMnAs (0.881)
$Fe_2Mo_3O_8$ (0.331)	Fe_2O_3 (0.299)	Fe_2O_3 (0.300)	Fe_2O_3-alpha (0.65)	Fe_2PO_5 (0.263)
Fe_2SiO_4 (0.1071)	Fe_2WO_6 (0.811)	Fe_2WO_6 (0.813)	Fe_2WO_6 (0.814)	$Fe_3(PO_4)_2$ (0.264)
$Fe_3(PO_4)_2(OH)_2$ (0.392)	$Fe_3F_8(H_2O)_2$ (0.582)	$Fe_4Nb_2O_9$ (0.441)	$Fe_4Nb_2O_9$ (0.443)	$FeBO_3$ (0.112)
FeF_3 (0.335)	FeF_3 (0.581)	$FeOHSO_4$ (0.760)	FeOOH (0.399)	$FeSO_4F$ (0.128)
$GaFeO_3$ (0.38)	$InCrO_3$ (0.308)	K_2ReI_6 (0.434)	K_2ReI_6 (0.553)	$KFeS_2$ (0.633)
$KMnF_3$ (0.432)	La_2LiRuO_6 (0.148)	$LaBaMn_2O_5$ (0.735)	$LaCrO_3$ (0.323)	$LaCrO_3$ (0.417)
$LaMnO_3$ (0.1)	$LaMnO_3$ (0.642)	$Li_2Co(SO_4)_2$ (0.121)	$Li_2Mn(SO_4)_2$ (0.122)	$Li_2Ni(SO_4)_2$ (0.714)
$LiCrGe_2O_6$ (0.217)	$LiCrGe_2O_6$ (0.961)	$LiCrGe_2O_6$ (0.962)	$LiCrGe_2O_6$ (0.963)	$LiCrGe_2O_6$ (0.964)
$LiFeP_2O_7$ (0.83)	$LiFeSi_2O_6$ (0.28)	$LiMn_6Sn_6$ (0.699)	$LiMnPO_4$ (0.24)	$LiMnPO_4$ (0.382)
$LuCrO_3$ (0.1068)	$LuCrWO_6$ (0.1082)	$LuFeO_3$ (0.117)	$LuVO_3$ (0.984)	$Mn(N(CN_2))_2$ (0.131)
Mn_2FeReO_6 (0.541)	$Mn_2Mo_3O_8$ (0.333)	Mn_2Sb (0.855)	$Mn_2SeO_3F_2$ (0.755)	Mn_3AlN (0.275)
Mn_3AlN (0.276)	Mn_3As_2 (0.512)	Mn_3As (0.279)	Mn_3As (0.280)	Mn_3Ge (0.377)
Mn_3Ir (0.108)	Mn_3IrGe (0.1006)	Mn_3Pt (0.109)	Mn_3Sn (0.199)	Mn_3Sn (0.200)
Mn_3Sn_2 (0.662)	$Mn_3Ti_2Te_6$ (0.176)	Mn_4N (0.274)	$Mn_4Nb_2O_9$ (0.507)	$Mn_4Ta_2O_9$ (0.477)
$Mn_4Ta_2O_9$ (0.526)	Mn_5Ge_3 (0.286)	$MnCO_3$ (0.115)	MnCoGe (0.445)	$MnGeN_2$ (0.1065)
$MnGeO_3$ (0.312)	$MnLaMnSbO_6$ (0.234)	$MnNb_2O_6$ (0.815)	$MnPS_3$ (0.163)	$MnPSe_3$ (0.180)
$MnPSe_3$ (0.524)	$MnPd_2$ (0.798)	$MnSiN_2$ (0.1066)	$MnTa_2O_6$ (0.816)	$MnTiO_3$ (0.19)
$MnTiO_3$ (0.50)	$Na_2BaCo(VO_4)_2$ (0.266)	$NaCrGe_2O_6$ (0.297)	$NaMnFeF_6$ (0.310)	$NaOsO_3$ (0.25)
$NiCO_3$ (0.113)	$NiCr_2O_4$ (0.4)	$NiCr_2O_4$ (0.895)	NiF_2 (0.36)	$NiFePO_5$ (0.261)
$RbFe_2F_6$ (0.192)	$RbFeS_2$ (0.636)	$ScCrO_3$ (0.307)	$ScMnO_3$ (0.7)	Sr_2CoOsO_6 (0.210)
Sr_2CoTeO_6 (0.301)	Sr_2CoTeO_6 (0.937)	$Sr_2Fe_2O_5$ (0.1084)	Sr_2LuRuO_6 (0.420)	Sr_2MnGaO_5 (0.823)
Sr_2MnTeO_6 (0.936)	Sr_2NiTeO_6 (0.934)	Sr_2ScOsO_6 (0.917)	Sr_2YRuO_6 (0.795)	$Sr_4Fe_4O_{11}$ (0.402)
$SrMnO_3$ (0.1018)	$SrMnO_3$ (0.1019)	$SrRuO_3$ (0.732)	$Tl_3Fe_2S_4$ (0.801)	$TlCrO_3$ (0.309)
V_2WO_6 (0.966)	$Y_2Cu_2O_5$ (0.241)	$YBaMn_2O_5$ (0.739)	YCo_3 (0.859)	$YCrO_3$ (0.586)
$YCrO_3$ (0.947)	YNi_4Si (0.374)	$YRuO_3$ (0.513)	YVO_3 (0.787)	$ZrMn_2Ge_4O_{12}$ (0.315)

B. First-Principles Total-Energy Calculations

For these 253 materials whose magnetic structures are included in the initial set of magnetic configurations from our irrep basis-vector strategy, the first-principles total-energy calculations were performed, using the Vienna *ab initio* Simulation Package (VASP) [12, 13]. The calculations employ a spin-polarized GGA + SOC + U approach. The on-site Coulomb interaction parameters U and J are chosen as the averaged values recommended for transition-metal elements based on the linear-response scheme [14]. We further verify that reasonable variations of U within physically relevant ranges do not alter the predicted magnetic structure.

Our DFT calculations successfully reproduce 198 out of 253 magnetic structures, yielding a total accuracy of 78.2%, as summarized in Table S9.

TABLE S9. Table of first-principles benchmark results based on well-selected input structures. Among the 253 materials subjected to first-principles calculations, the magnetic structure obtained from DFT agree with experimental results in 198 cases, whereas deviations from experimental results are found in the remaining 55 cases, which may arise from the intrinsic limitations of DFT. Material names are followed by their corresponding labels (in parentheses) from the MAGNDATA database[32].

	Materials				
Our framework successfully predict the experimental magnetic ground states for these materials	$AlFe_2B_2$ (0.414)	$Ba_2CoGe_2O_7$ (0.56)	$Ba_2MnSi_2O_7$ (0.229)	$Ba_3NiRu_2O_9$ (0.748)	$BaCr_2As_2$ (0.365)
	$BaCrF_5$ (0.303)	$BaCuF_4$ (0.191)	$BaFe_2S_2O$ (0.987)	$BaMn_2As_2$ (0.18)	$BaMn_2Bi_2$ (0.89)
	$BaMn_2Ge_2$ (0.605)	$BaMn_2Ge_2$ (0.606)	$BaMn_2P_2$ (0.464)	$BaMn_2Sb_2$ (0.470)	$BaMnSb_2$ (0.611)
	$BaNi_2P_2O_8$ (0.215)	Bi_2CuO_4 (0.348)	Bi_2CuO_4 (0.694)	Bi_2CuO_4 (0.695)	$BiCrO_3$ (0.138)
	$Ca_2Fe_2O_5$ (0.1080)	Ca_2FeOsO_6 (0.682)	Ca_2NiOsO_6 (0.796)	$CaCu_3Fe_2Sb_2O_{12}$ (0.672)	$CaFe_5O_7$ (0.358)
	$CaIrO_3$ (0.79)	$CaMn_2Ge_2$ (0.603)	$CaMn_2Ge_2$ (0.604)	$CaMn_2Sb_2$ (0.92)	$CaMnBi_2$ (0.72)
	$CaMnGe_2O_6$ (0.156)	CaMnSi (0.599)	CaMnSi (0.600)	$Co_2Mo_3O_8$ (0.332)	$Co_2Mo_3O_8$ (0.338)
	$Co_3Sn_2S_2$ (0.860)	$Co_3Sn_2S_2$ (0.861)	$Co_4Nb_2O_9$ (0.111)	$CoCO_3$ (0.114)	CoF_2 (0.178)
	CoF_3 (0.334)	$CoSe_2O_5$ (0.161)	$CoTa_4Se_8$ (0.1036)	Cr_2O_3 (0.110)	Cr_2O_3 (0.59)
	Cr_2TeO_6 (0.143)	Cr_2TeO_6 (0.76)	Cr_2TeO_6 (0.959)	Cr_2WO_6 (0.144)	Cr_2WO_6 (0.75)
	CrSb (0.528)	$CrSbSe_3$ (0.834)	$CuFePO_5$ (0.260)	$CuFeS_2$ (0.802)	CuMnAs (0.222)
	CuMnAs (0.881)	$Fe_2Mo_3O_8$ (0.331)	Fe_2O_3-alpha (0.65)	Fe_2PO_5 (0.263)	Fe_2SiO_4 (0.1071)
	Fe_2TeO_6 (0.142)	Fe_2TeO_6 (0.960)	Fe_2WO_6 (0.814)	$Fe_3(PO_4)_2(OH)_2$ (0.392)	$Fe_3F_8(H_2O)_2$ (0.582)
	$FeBO_3$ (0.112)	$FeCO_3$ (0.116)	FeF_3 (0.335)	FeF_3 (0.581)	$FeOHSO_4$ (0.760)
	FeOOH (0.399)	$FeSO_4F$ (0.128)	$GaFeO_3$ (0.38)	$InCrO_3$ (0.308)	K_2ReI_6 (0.434)
	K_2ReI_6 (0.553)	$KFeS_2$ (0.633)	$KFeSe_2$ (0.637)	KMnBi (0.618)	$KMnF_3$ (0.432)
	$KMnF_3$ (0.433)	KMnSb (0.617)	$KOsO_4$ (0.284)	$KRuO_4$ (0.285)	La_2LiRuO_6 (0.148)
	$La_2O_3Mn_2Se_2$ (0.1092)	$La_2O_3Mn_2Se_2$ (0.1093)	$LaBaMn_2O_6$ (0.737)	$LaBaMn_2O_6$ (0.738)	$LaCrO_3$ (0.323)
	$LaCrO_3$ (0.416)	$LaCrO_3$ (0.417)	$LaMn_2Si_2$ (0.472)	$LaMn_2Si_2$ (0.498)	LaMnAsO (0.619)
	LaMnAsO (0.624)	LaMnSbO (0.667)	$Li_2Co(SO_4)_2$ (0.121)	$Li_2Mn(SO_4)_2$ (0.122)	$Li_2Ni(SO_4)_2$ (0.714)
	$LiCoPO_4$ (0.193)	$LiCoPO_4$ (0.383)	$LiFe_2F_6$ (0.501)	$LiFeP_2O_7$ (0.83)	$LiFePO_4$ (0.95)
	$LiMn_6Sn_6$ (0.699)	$LiMnPO_4$ (0.24)	$LiMnPO_4$ (0.382)	$LuCrO_3$ (0.1068)	$LuCrWO_6$ (0.1082)
	$Mn(N(CN_2))_2$ (0.131)	Mn_2Au (0.1081)	Mn_2Au (0.639)	Mn_2Au (0.640)	Mn_2FeReO_6 (0.541)
	Mn_2Sb (0.855)	Mn_3As_2 (0.512)	Mn_3GaN (0.177)	Mn_3Ge (0.377)	Mn_3Ir (0.108)
	Mn_3Sn (0.199)	Mn_3Sn (0.200)	$Mn_3Ti_2Te_6$ (0.176)	Mn_3ZnN (0.273)	Mn_4N (0.274)
	$Mn_4Nb_2O_9$ (0.507)	$Mn_4Ta_2O_9$ (0.477)	$Mn_4Ta_2O_9$ (0.526)	Mn_5Ge_3 (0.286)	$MnCO_3$ (0.115)
	MnF_2 (0.15)	$MnGeN_2$ (0.1065)	$MnGeO_3$ (0.125)	$MnGeO_3$ (0.312)	$MnLaMnSbO_6$ (0.234)
	$MnNb_2O_6$ (0.815)	$MnNb_4S_8$ (0.709)	$MnPS_3$ (0.163)	$MnPSe_3$ (0.180)	$MnPSe_3$ (0.524)
	$MnPd_2$ (0.798)	$MnSiN_2$ (0.1066)	$MnTa_2O_6$ (0.816)	$MnTa_4S_8$ (0.711)	MnTe (0.800)
	$MnTe_2$ (0.20)	$MnTiO_3$ (0.19)	$MnTiO_3$ (0.50)	$Na_2BaCo(VO_4)_2$(0.266)	$NaCrGe_2O_6$ (0.297)
	NaMnAs (0.629)	NaMnAs (0.630)	NaMnBi (0.634)	NaMnBi (0.635)	$NaMnFeF_6$ (0.310)
	NaMnP (0.626)	NaMnP (0.627)	NaMnP (0.628)	NaMnSb (0.631)	NaMnSb (0.632)
	$NaOsO_3$ (0.25)	$NiCO_3$ (0.113)	$NiCr_2O_4$ (0.4)	$NiCrO_4$ (0.896)	NiF_2 (0.36)
	$NiFePO_5$ (0.261)	NiS_2 (0.150)	$PbNiO_3$ (0.21)	$RbFe_2F_6$ (0.192)	$RbFeS_2$ (0.636)
	$RbFeSe_2$ (0.638)	RuO_2 (0.607)	$ScCrO_3$ (0.307)	Sr_2CoTeO_6 (0.301)	Sr_2CoTeO_6 (0.937)
	Sr_2LuRuO_6 (0.420)	Sr_2MnGaO_5 (0.823)	Sr_2MnTeO_6 (0.936)	Sr_2NiTeO_6 (0.934)	Sr_2ScOsO_6 (0.917)
	Sr_2YRuO_6 (0.795)	$Sr_4Fe_4O_{11}$ (0.401)	$Sr_4Fe_4O_{11}$ (0.402)	$SrCr_2As_2$ (0.364)	$SrMn_2As_2$ (0.482)
	$SrMnBi_2$ (0.73)	$SrMnO_3$ (0.1018)	$SrMnO_3$ (0.1019)	$SrRuO_3$ (0.732)	$TlCrO_3$ (0.309)
	V_2WO_6 (0.966)	VNb_3S_6 (0.712)	$Y_2Cu_2O_5$ (0.241)	$YCrO_3$ (0.586)	$YCrO_3$ (0.947)
	YVO_3 (0.787)	$ZrMn_2Ge_4O_{12}$ (0.315)	$[Na(OH)_2]_3Mn(NCS)_3$ (0.1078)		
Our framework failed to identify the experimental magnetic ground state for these materials	$Ba_2Mn_3Sb_2O_2$ (0.471)	Ca_2MnGaO_5 (0.825)	$CaFe_2O_4$ (0.968)	$CaFe_2O_4$ (0.969)	$CaFe_4Al_8$ (0.236)
	Cr_2CoAl (0.1073)	Cr_2MoO_6 (0.1023)	$CrNb_4S_8$ (0.708)	$CsMnF_4$ (0.327)	Fe_2O_3 (0.299)
	Fe_2O_3 (0.300)	Fe_2WO_6 (0.811)	Fe_2WO_6 (0.813)	$Fe_3(PO_4)_2$ (0.264)	$Fe_4Nb_2O_9$ (0.441)
	$Fe_4Nb_2O_9$ (0.443)	$La_2O_3Mn_2Se_2$ (0.1091)	$LaBaMn_2O_5$ (0.735)	$LaMnO_3$ (0.1)	$LaMnO_3$ (0.642)
	$LaMnSi_2$ (0.778)	$LaMnSi_2$ (0.779)	$LaMnSi_2$ (0.780)	$LiCrGe_2O_6$ (0.217)	$LiCrGe_2O_6$ (0.961)
	$LiCrGe_2O_6$ (0.962)	$LiCrGe_2O_6$ (0.963)	$LiCrGe_2O_6$ (0.964)	$LiFeSi_2O_6$ (0.28)	$LuFeO_3$ (0.117)
	$LuVO_3$ (0.984)	$MgMnO_3$ (0.277)	$Mn_2Mo_3O_8$ (0.333)	$Mn_2SeO_3F_2$ (0.755)	Mn_3AlN (0.275)
	Mn_3AlN (0.276)	Mn_3As (0.279)	Mn_3As (0.280)	Mn_3IrGe (0.1006)	Mn_3Pt (0.109)
	Mn_3Sn_2 (0.662)	MnCoGe (0.445)	MnPtGa (0.395)	$NiCr_2O_4$ (0.895)	$ScMnO_3$ (0.7)
	Sr_2CoOsO_6 (0.210)	$Sr_2Fe_2O_5$ (0.1084)	$Sr_2Mn_3As_2O_2$ (0.212)	$SrMnSb_2$ (0.767)	$Tl_3Fe_2S_4$ (0.801)
	$YBaMn_2O_5$ (0.739)	YCo_3 (0.859)	$YMnO_3$ (0.6)	YNi_4Si (0.374)	$YRuO_3$ (0.513)

III. MAGNETIC MATERIALS DATABASE

A. Statistics of Magnetic Materials

We applied our framework to the Inorganic Crystal Structure Database (ICSD) [58]. After excluding entries with fractional site occupancies, we focus on the materials with fewer than 30 atoms in the unit cell and exclude lanthanoids and actinoids due to the challenges in accurately described within standard density functional theory [33]. To limit the computational cost at this stage, we consider the magnetic structures with a propagation vector $\mathbf{q} = 0$, and performed systematic high-throughput first-principles calculations to determine the magnetic structure of 8,422 transition-metal compounds. Within this well-defined scope, our workflow identified 5,516 materials as non-magnetic. The remaining 2,906 magnetic materials were compiled into a magnetic structure database. Calculations for materials exceeding 30 atoms per unit cell are currently in progress. The magnetic structure, electronic band structures, and associated information of topological magnetic materials is available at `https://magdatabase.nju.edu.cn`, which is continuously updated. The corresponding magCIF files are also available for download on the website for user access.

This database captures a broad diversity of magnetic configurations. From the viewpoint of magnetic classification, 1,449 materials exhibit ferromagnetic (FM) ordering, and 338 materials are classified as ferrimagnetic (FiM). 1,119 compounds exhibit antiferromagnetic (AFM) order with vanishing net magnetization, including 392 altermagnets. Ferromagnetic materials, collinear ferrimagnetic materials, non-collinear ferrimagnetic materials, collinear antiferromagnetic materials, non-collinear antiferromagnetic materials, and altermagnetic materials are in Table S10-S32, S33-S36, S37-S38, S39-S48, S49-S50, S51-S57, respectively.

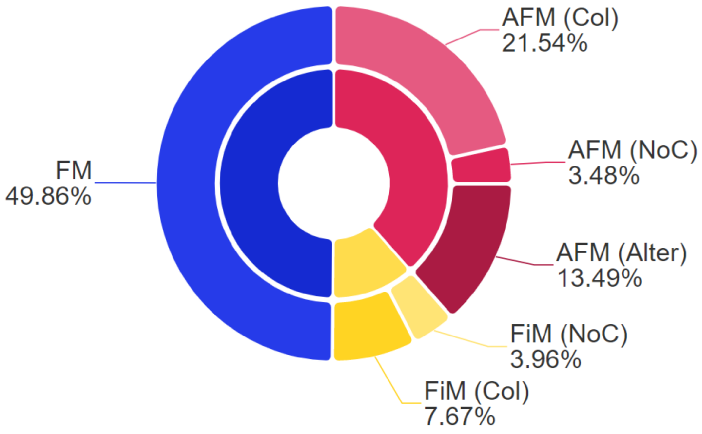


FIG. S3. **Magnetic and topological classification of our magnetic structure database.** (a) Statistics of magnetic ground-state classification.Among the 2,906 identified magnetic materials, 49.86% exhibit ferromagnetic (FM) ordering, 11.63% are ferrimagnetic (FiM), and the remaining 38.51% are antiferromagnetic (AFM).The FiM materials are further classified into 7.67% collinear (Col) and 3.96% noncollinear (NoC) states according to the relative orientation of magnetic moments.Within the AFM materials, 21.54% exhibit collinear (Col) order, 3.48% exhibit noncollinear (NoC) order, and 13.49% are classified as altermagnets (Alter).

B. Ferromagnetic Materials

The relevant information for the ferromagnetic materials is summarized in Table S10-S32, including their chemical formula, space group, magnetic space group, band gap and corresponding irreducible representations of crystallographic space group.

TABLE S10. Tabulated information on **ferromagnetic** materials, including the chemical formula, space group, magnetic space group, band gap and corresponding irreducible representations of crystallographic space group.

ICSD number	Chemical formula	SG NUM	BNS	Band Gap (eV)	Irrep
icsd_079879	$AgBi_2F_{12}$	2	2.4	0.80	Γ_1^+
icsd_065186	$AgF_{12}Sb_2$	2	2.4	0.90	Γ_1^+
icsd_051505	AgF_6Sn	2	2.4	0.71	Γ_1^+
icsd_051506	AgF_6Ti	2	2.4	0.11	Γ_1^+
icsd_063058	$As_2CuNa_4O_8$	2	2.4	2.41	Γ_1^+
icsd_018115	$As_2CuO_8Zn_2$	2	2.4	2.17	Γ_1^+
icsd_062544	$AuCuF_5$	2	2.4	1.89	Γ_1^+
icsd_174291	Ba_2BiIrO_6	2	2.4	0.40	Γ_1^+
icsd_174140	Ba_2IrLaO_6	2	2.4	0.33	Γ_1^+
icsd_037027	Ba_2LaO_6Ru	2	2.4	1.19	Γ_1^+
icsd_246513	$BaMn_2O_6Y$	2	2.4	0.00	Γ_1^+
icsd_424465	$Br_{10}CoY_6$	2	2.4	0.01	Γ_1^+
icsd_423462	Br_5W	2	2.4	0.25	Γ_1^+
icsd_172335	$C_2CuF_6O_6S_2$	2	2.4	2.19	Γ_1^+
icsd_099499	$C_6CuFeK_2N_6$	2	2.4	1.11	Γ_1^+
icsd_171007	$Ca_2Cl_2CuO_{10}Te_4$	2	2.4	2.06	Γ_1^+
icsd_249777	$Cd_2CuO_8P_2$	2	2.4	2.21	Γ_1^+
icsd_074682	$Cl_{12}OsTe_2$	2	2.4	0.67	Γ_1^+
icsd_068656	$Cl_{12}ReTe_2$	2	2.4	0.82	Γ_1^+
icsd_066023	$Cl_{12}Te_4W_2$	2	2.4	0.08	Γ_1^+
icsd_084620	Cl_5Mo	2	2.4	0.43	Γ_1^+
icsd_078789	Cl_6ISe_6W	2	2.4	0.36	Γ_1^+
icsd_415768	Cl_8NW_2	2	2.4	0.43	Γ_1^+
icsd_099580	$Co_2Na_6O_6$	2	2.4	1.98	Γ_1^+
icsd_424841	$CoI_{10}Y_6$	2	2.4	0.00	Γ_1^+
icsd_092852	$CoLi_2O_8W_2$	2	2.4	2.92	Γ_1^+
icsd_062676	$CrNa_4O_4$	2	2.4	1.16	Γ_1^+
icsd_050444	$Cs_4CuO_7Si_2$	2	2.4	2.02	Γ_1^+
icsd_409506	$Cs_6NiO_8Si_2$	2	2.4	1.92	Γ_1^+
icsd_078869	$CuF_{11}NaZr_2$	2	2.4	3.80	Γ_1^+
icsd_064660	CuF_6Pt	2	2.4	1.71	Γ_1^+
icsd_036514	CuF_6Sn	2	2.4	3.37	Γ_1^+
icsd_030117	CuF_6Zr	2	2.4	3.49	Γ_1^+
icsd_200533	$CuFNbO_3$	2	2.4	2.35	Γ_1^+
icsd_085404	$CuK_6O_8Si_2$	2	2.4	1.96	Γ_1^+
icsd_092854	$CuLi_2O_8W_2$	2	2.4	2.03	Γ_1^+
icsd_002896	$CuO_6S_2Tl_2$	2	2.4	1.13	Γ_1^+
icsd_028151	CuO_6V_2	2	2.4	1.63	Γ_1^+
icsd_085405	$CuO_7Rb_4Si_2$	2	2.4	2.09	Γ_1^+
icsd_411522	$F_{12}MnSb_2$	2	2.4	3.69	Γ_1^+
icsd_171656	F_6O_2Rh	2	2.4	0.00	Γ_1^+
icsd_059585	$FeNa_4O_4$	2	2.4	0.59	Γ_1^+
icsd_184601	$FLiO_4PV$	2	2.4	2.03	Γ_1^+
icsd_068184	H_2CuO_5S	2	2.4	2.07	Γ_1^+
icsd_039887	H_2CuO_5Se	2	2.4	2.33	Γ_1^+
icsd_069994	H_2O_5SeV	2	2.4	2.39	Γ_1^+
icsd_156225	$H_4Ca_2MnO_{10}P_2$	2	2.4	4.22	Γ_1^+
icsd_098686	$H_4CoK_2O_{10}Se_2$	2	2.4	3.74	Γ_1^+
icsd_098683	$H_4CoNa_2O_{10}Se_2$	2	2.4	3.54	Γ_1^+
icsd_087958	$H_4FeK_2O_{10}S_2$	2	2.4	3.99	Γ_1^+
icsd_096783	$H_4K_2MnO_{10}Se_2$	2	2.4	3.25	Γ_1^+
icsd_098684	$H_4Na_2NiO_{10}Se_2$	2	2.4	3.44	Γ_1^+
icsd_072461	$H_6CuN_4O_4$	2	2.4	1.39	Γ_1^+
icsd_280299	$H_8CdCl_4CuO_4$	2	2.4	1.59	Γ_1^+
icsd_080430	$KMnO_8Se_2$	2	2.4	1.43	Γ_1^+
icsd_077829	$LaSe$	2	2.4	0.00	Γ_1^+
icsd_092853	$Li_2NiO_8W_2$	2	2.4	2.90	Γ_1^+
icsd_189335	MoO_6Sr_2Ti	2	2.4	0.00	Γ_1^+
icsd_260257	$NiO_{10}Te_2V_2$	2	2.4	2.00	Γ_1^+
icsd_001501	O_2V	2	2.4	0.00	Γ_1^+
icsd_415445	O_5PSnV	2	2.4	1.10	Γ_1^+
icsd_099699	$BaMn_2O_6Y$	3	3.3	0.00	Γ_2
icsd_670113	$CuFO_2$	4	4.7	0.74	Γ_1
icsd_093022	O_7P_2V	4	4.9	1.69	Γ_2
icsd_068143	AgP_2Se_6V	5	5.13	0.39	Γ_1

TABLE S11. Tabulated information on **ferromagnetic** materials, including the chemical formula, space group, magnetic space group, band gap and corresponding irreducible representations of crystallographic space group.

ICSD number	Chemical formula	SG NUM	BNS	Band Gap (eV)	Irrep
icsd_075180	As_2FeLiO_7	5	5.13	2.54	Γ_1
icsd_084683	B_2BaCuO_5	5	5.15	2.22	Γ_2
icsd_046003	CoO_6V_2	5	5.15	2.28	Γ_2
icsd_260893	$CrCsP_2S_7$	5	5.15	1.68	Γ_2
icsd_091754	$CrKP_2S_7$	5	5.15	1.70	Γ_2
icsd_059910	CsP_2S_7V	5	5.15	1.54	Γ_2
icsd_021067	CuO_6V_2	5	5.13	1.25	Γ_1
icsd_039871	$HCsMnO_{10}P_3$	5	5.15	1.13	Γ_2
icsd_091756	KP_2S_7V	5	5.15	1.50	Γ_2
icsd_073782	P_2RbS_7V	5	5.15	1.52	Γ_2
icsd_068713	S_2V	5	5.13	0.00	Γ_1
icsd_168320	$BiFeO_3$	8	8.34	1.49	Γ_2
icsd_095439	Ca_2CoO_3	8	8.34	0.00	Γ_2
icsd_006179	$CCuO_3$	8	8.34	0.00	Γ_2
icsd_095440	CoO_2	8	8.34	1.37	Γ_2
icsd_023476	$CrNb_2Se_4$	8	8.34	0.00	Γ_2
icsd_169981	$HNiO_2$	8	8.32	0.00	Γ_1
icsd_645393	Nb_2Se_4Ti	8	8.34	0.00	Γ_2
icsd_645398	Nb_2Se_4V	8	8.32	0.00	Γ_1
icsd_023174	$CaCrF_5$	9	9.37	2.22	Γ_1
icsd_169098	MoO_5P	9	9.37	0.12	Γ_1
icsd_150279	$AuCrTe_4$	10	10.42	0.00	Γ_1^+
icsd_028909	CrO_3Y	10	10.46	1.20	Γ_2^+
icsd_001503	O_2V	10	10.46	0.00	Γ_2^+
icsd_089471	O_2V	10	10.46	1.07	Γ_2^+
icsd_246090	Ca_2MnO_6Sb	11	11.54	0.00	Γ_2^+
icsd_246091	Ca_2MnO_6Ta	11	11.54	0.00	Γ_2^+
icsd_084827	$CoHf_2P$	11	11.54	0.00	Γ_2^+
icsd_018176	CoO_4S	11	11.54	0.00	Γ_2^+
icsd_002232	CuI_2O_6	11	11.50	2.15	Γ_1^+
icsd_170771	$MnNaO_4Rb_2$	11	11.54	1.91	Γ_2^+
icsd_172559	Ag_2NiO_2	12	12.58	0.00	Γ_1^+
icsd_670065	$AgMnO_2$	12	12.62	0.31	Γ_2^+
icsd_670103	$AuCuO_2$	12	12.62	0.00	Γ_2^+
icsd_670093	$AuMnO_2$	12	12.62	0.00	Γ_2^+
icsd_015079	B_4Mn	12	12.62	0.00	Γ_2^+
icsd_021055	Ba_2CuF_6	12	12.62	2.18	Γ_2^+
icsd_174141	Ba_2IrLaO_6	12	12.58	0.38	Γ_1^+
icsd_023903	Br_2Cr	12	12.62	1.08	Γ_2^+
icsd_022079	Br_2Cu	12	12.62	0.26	Γ_2^+
icsd_250692	$C_2CoN_2S_2$	12	12.58	1.83	Γ_1^+
icsd_031320	$C_2N_2NiS_2$	12	12.62	1.61	Γ_2^+
icsd_617514	$C_3Cr_2Lu_2$	12	12.62	0.00	Γ_2^+
icsd_617562	$C_3Cr_2Y_2$	12	12.62	0.00	Γ_2^+
icsd_160557	Ca_2CoO_3	12	12.58	0.00	Γ_1^+
icsd_670347	$CaMnO_3$	12	12.62	0.00	Γ_2^+
icsd_026667	Cl_2Cu	12	12.62	0.97	Γ_2^+
icsd_022080	Cl_3Cr	12	12.62	2.17	Γ_2^+
icsd_403035	Cl_4CrLi_2	12	12.62	1.40	Γ_2^+
icsd_623661	$Co_2Ge_4Y_3$	12	12.58	0.00	Γ_1^+
icsd_099989	Co_3Se_4	12	12.62	0.00	Γ_2^+
icsd_623472	$CoGe_2Lu_2$	12	12.58	0.00	Γ_1^+
icsd_017013	CoO	12	12.58	1.85	Γ_1^+
icsd_160556	CoO_2	12	12.62	1.33	Γ_2^+
icsd_099894	CoO_3Sr_2	12	12.62	0.00	Γ_2^+
icsd_169194	CoO_6Pb_2Te	12	12.62	1.22	Γ_2^+
icsd_077912	CoO_6Pb_2W	12	12.58	1.87	Γ_1^+
icsd_188911	CoO_6V_2	12	12.62	2.25	Γ_2^+
icsd_624816	$CoRh_2Se_4$	12	12.62	0.00	Γ_2^+
icsd_041746	$CoSc_2Si_2$	12	12.58	0.00	Γ_1^+
icsd_624999	$CoSe_4Si_2$	12	12.62	0.00	Γ_2^+
icsd_002371	$CoSi_2Zr_2$	12	12.58	0.00	Γ_1^+
icsd_014026	$Cr_{0.5}NbSe_2$	12	12.62	0.00	Γ_2^+
icsd_626279	Cr_2MnS_4	12	12.58	0.00	Γ_1^+
icsd_626299	Cr_2MnSe_4	12	12.62	0.00	Γ_2^+

TABLE S12. Tabulated information on **ferromagnetic** materials, including the chemical formula, space group, magnetic space group, band gap and corresponding irreducible representations of crystallographic space group.

ICSD number	Chemical formula	SG NUM	BNS	Band Gap (eV)	Irrep
icsd_626640	Cr_2S_4Ti	12	12.62	0.00	Γ_2^+
icsd_626896	Cr_2Te_4Ti	12	12.62	0.00	Γ_2^+
icsd_626901	Cr_2Te_4V	12	12.62	0.00	Γ_2^+
icsd_016722	Cr_3S_4	12	12.62	0.00	Γ_2^+
icsd_026976	Cr_3Se_4	12	12.58	0.00	Γ_1^+
icsd_626873	Cr_3Te_4	12	12.58	0.00	Γ_1^+
icsd_169764	CrF_3K	12	12.62	1.11	Γ_2^+
icsd_151873	$CrFe_2Se_4$	12	12.58	0.00	Γ_1^+
icsd_004073	CrI_2	12	12.58	0.54	Γ_1^+
icsd_251654	CrI_3	12	12.62	0.62	Γ_2^+
icsd_626521	$CrPSe_3$	12	12.58	0.00	Γ_1^+
icsd_626577	$CrRh_2Se_4$	12	12.62	0.00	Γ_2^+
icsd_626579	$CrRh_2Te_4$	12	12.62	0.00	Γ_2^+
icsd_075420	CrS_2	12	12.62	0.00	Γ_2^+
icsd_251718	$CrSe_2$	12	12.62	0.00	Γ_2^+
icsd_072287	Cs_4IrO_4	12	12.62	0.58	Γ_2^+
icsd_066509	$Cu_2Li_3O_4$	12	12.62	0.00	Γ_2^+
icsd_670115	$CuHgO_2$	12	12.62	0.47	Γ_2^+
icsd_174134	$CuLi_2O_2$	12	12.62	0.38	Γ_2^+
icsd_030379	$CuMnO_2$	12	12.62	0.04	Γ_2^+
icsd_096699	CuO_2	12	12.58	0.00	Γ_1^+
icsd_633517	Fe_2Se_4V	12	12.58	0.00	Γ_1^+
icsd_427606	$FeLa_2O_2Se_2$	12	12.62	2.31	Γ_2^+
icsd_022085	$H_4Br_2CoO_2$	12	12.58	2.48	Γ_1^+
icsd_022084	$H_4Br_2MnO_2$	12	12.58	3.00	Γ_1^+
icsd_022082	$H_4Cl_2CoO_2$	12	12.58	3.16	Γ_1^+
icsd_015597	$H_4Cl_2FeO_2$	12	12.62	3.20	Γ_2^+
icsd_015596	$H_4Cl_2MnO_2$	12	12.58	4.07	Γ_1^+
icsd_009485	$H_4CuF_2O_2$	12	12.62	3.16	Γ_2^+
icsd_260368	$H_4O_{10}V_4$	12	12.58	1.07	Γ_1^+
icsd_047223	IrK_4O_4	12	12.62	0.74	Γ_2^+
icsd_016270	$MnNaO_2$	12	12.62	0.99	Γ_2^+
icsd_150462	MnO_2	12	12.62	0.51	Γ_2^+
icsd_040850	MnO_6V_2	12	12.62	1.63	Γ_2^+
icsd_201787	Mo_2S_4V	12	12.62	0.00	Γ_2^+
icsd_026609	$NaNiO_2$	12	12.58	0.16	Γ_1^+
icsd_182323	NaO_2V	12	12.58	1.83	Γ_1^+
icsd_076548	$NaSe_2V$	12	12.62	0.29	Γ_2^+
icsd_645395	Nb_2Se_4Ti	12	12.62	0.00	Γ_2^+
icsd_645402	Nb_2Se_4V	12	12.58	0.00	Γ_1^+
icsd_076670	NiO	12	12.62	1.75	Γ_2^+
icsd_016225	NiO_6Sr_2Te	12	12.62	2.10	Γ_2^+
icsd_015214	$NiRh_2Se_4$	12	12.62	0.00	Γ_2^+
icsd_646533	$NiSe_4Si_2$	12	12.62	0.00	Γ_2^+
icsd_084195	Se_4V_3	12	12.62	0.00	Γ_2^+
icsd_038369	$Te_2V_{1.04}$	12	12.58	0.00	Γ_1^+
icsd_653087	Te_4TiV_2	12	12.58	0.00	Γ_1^+
icsd_052510	Te_4V_3	12	12.62	0.00	Γ_2^+
icsd_246938	$BaCoS_2$	13	13.69	0.00	Γ_2^+
icsd_169005	CuO_4W	13	13.65	1.16	Γ_1^+
icsd_170685	MnO_4Re	13	13.69	0.00	Γ_2^+
icsd_093880	$AgCuO_2$	14	14.75	0.00	Γ_1^+
icsd_421461	AgF_4K_2	14	14.79	0.98	Γ_2^+
icsd_153857	Bi_2MnNiO_6	14	14.75	0.27	Γ_1^+
icsd_290790	Ca_2CrO_6Sb	14	14.79	1.68	Γ_2^+
icsd_150696	Ca_2FeO_6Re	14	14.75	0.00	Γ_1^+
icsd_247998	Ca_2MnO_6Re	14	14.79	0.00	Γ_2^+
icsd_084791	Ca_3O_6Re	14	14.79	0.00	Γ_2^+
icsd_092336	$CaFeO_3$	14	14.79	0.00	Γ_2^+
icsd_182568	CaO_6ReSr_2	14	14.75	0.00	Γ_1^+
icsd_066201	Cl_4CrNa_2	14	14.79	1.61	Γ_2^+
icsd_151837	$CoLa_2MnO_6$	14	14.79	0.00	Γ_2^+
icsd_188982	$CoMnO_6Y_2$	14	14.75	1.15	Γ_1^+
icsd_173491	CoO_6ReSr_2	14	14.79	0.00	Γ_2^+
icsd_097662	CoO_6Sr_2W	14	14.79	2.10	Γ_2^+

TABLE S13. Tabulated information on **ferromagnetic** materials, including the chemical formula, space group, magnetic space group, band gap and corresponding irreducible representations of crystallographic space group.

ICSD number	Chemical formula	SG NUM	BNS	Band Gap (eV)	Irrep
icsd_042614	$CoSb_2$	14	14.75	0.00	Γ_1^+
icsd_067250	CrF_4Na_2	14	14.79	2.06	Γ_2^+
icsd_010350	CrF_6Li_2	14	14.75	1.11	Γ_1^+
icsd_027070	CrF_6Na_3	14	14.79	3.54	Γ_2^+
icsd_191374	$CrMnO_6Y_2$	14	14.79	0.21	Γ_2^+
icsd_290789	CrO_6SbSr_2	14	14.75	1.10	Γ_1^+
icsd_096085	$CuGeO_3$	14	14.75	1.74	Γ_1^+
icsd_062655	F_4LiMn	14	14.79	2.09	Γ_2^+
icsd_071455	F_4MnNa	14	14.79	2.31	Γ_2^+
icsd_290251	F_6Li_2V	14	14.75	2.69	Γ_1^+
icsd_066315	F_6MnNa_3	14	14.79	1.66	Γ_2^+
icsd_026073	F_6Na_3Ni	14	14.79	2.20	Γ_2^+
icsd_027347	F_6Na_3V	14	14.79	2.50	Γ_2^+
icsd_095517	FeO_6Sr_2W	14	14.79	1.35	Γ_2^+
icsd_237528	In_2MnNiO_6	14	14.79	1.74	Γ_2^+
icsd_203219	La_2LiMoO_6	14	14.79	0.51	Γ_2^+
icsd_186428	La_2MnNiO_6	14	14.79	0.15	Γ_2^+
icsd_163761	La_2MnO_6V	14	14.79	1.20	Γ_2^+
icsd_054919	$LaMnO_3$	14	14.79	0.00	Γ_2^+
icsd_092051	$LuNiO_3$	14	14.79	0.35	Γ_2^+
icsd_151888	$Mn_{0.5}Ni_{0.5}O_3Y$	14	14.79	1.78	Γ_2^+
icsd_251832	$MnNiO_6Sc_2$	14	14.79	1.99	Γ_2^+
icsd_192872	$MnNiO_6Y_2$	14	14.79	0.96	Γ_2^+
icsd_251022	MnO_3Sc	14	14.75	0.91	Γ_1^+
icsd_069801	MnO_6Se_2	14	14.75	1.56	Γ_1^+
icsd_095948	NiO_3Tl	14	14.79	0.00	Γ_2^+
icsd_088043	NiO_3Y	14	14.79	0.23	Γ_2^+
icsd_150258	$LaMnO_3$	15	15.85	0.00	Γ_1^+
icsd_063230	BaS_3V	20	20.34	0.00	Γ_3
icsd_077832	S_2V	20	63.464	0.19	Γ_4
icsd_016834	$CuGeO_3$	26	51.296	0.00	Γ_3
icsd_041401	FeS_2	29	29.102	0.00	Γ_3
icsd_186518	FeO_4Si	31	31.125	0.00	Γ_4
icsd_002257	$HCrO_2$	31	31.125	2.02	Γ_4
icsd_088640	LiO_5V_2	31	31.125	1.52	Γ_4
icsd_047101	$MnNa_5O_4$	31	31.127	1.45	Γ_2
icsd_236365	MnO_3Y	31	31.125	0.49	Γ_4
icsd_001898	NaO_5V_2	31	31.125	1.52	Γ_4
icsd_042728	$CoTe_2$	34	34.159	0.00	Γ_2
icsd_042726	FeS_2	34	34.159	0.00	Γ_2
icsd_042727	$FeTe_2$	34	34.159	0.00	Γ_2
icsd_052692	BaS_3V	36	36.176	0.00	Γ_2
icsd_002596	CrI_2	36	36.174	0.00	Γ_4
icsd_068459	H_2CuO_2	36	36.176	1.81	Γ_2
icsd_000284	MgO_3V	36	36.174	2.78	Γ_4
icsd_617417	C_2CoLu	38	38.190	0.00	Γ_3
icsd_057007	C_2CoY	38	38.189	0.00	Γ_4
icsd_617756	C_2FeLu	38	38.191	0.00	Γ_2
icsd_050648	NbS_2	38	38.190	0.00	Γ_3
icsd_071339	$NbSe_2$	42	42.221	0.00	Γ_3
icsd_670101	$AgCuO_2$	47	47.252	0.00	Γ_4^+
icsd_085291	$Ba_2Cu_3LaO_8$	47	47.252	0.00	Γ_2^+
icsd_164176	$BaFe_2O_5Y$	47	47.252	0.05	Γ_4^+
icsd_095729	NbO	47	47.252	0.00	Γ_4^+
icsd_194435	$BNbRu$	51	51.294	0.00	Γ_2^+
icsd_421074	$Ca_2Ge_2Ni_3$	51	51.295	0.00	Γ_3^+
icsd_623100	Co_2GaLa	51	51.296	0.00	Γ_4^+
icsd_658677	Co_2InY	51	51.295	0.00	Γ_3^+
icsd_190616	Co_2NbSn	51	51.295	0.00	Γ_3^+
icsd_071520	$FeNbTe_2$	53	53.328	0.00	Γ_4^+
icsd_015087	$H_4Cl_2CuO_2$	53	53.328	2.03	Γ_4^+
icsd_083907	$CrLaSb_3$	57	57.383	0.00	Γ_3^+
icsd_610034	As_2Co	58	58.398	0.00	Γ_3^+
icsd_236413	$C_2H_2CoN_4$	58	58.397	2.24	Γ_2^+
icsd_172908	$C_2H_2N_4Ni$	58	58.398	2.53	Γ_4^+

TABLE S14. Tabulated information on **ferromagnetic** materials, including the chemical formula, space group, magnetic space group, band gap and corresponding irreducible representations of crystallographic space group.

ICSD number	Chemical formula	SG NUM	BNS	Band Gap (eV)	Irrep
icsd_015467	Cl_2Cr	58	58.398	1.41	Γ_3^+
icsd_076120	$CoSb_2$	58	58.398	0.00	Γ_3^+
icsd_042540	$CoSe_2$	58	58.397	0.00	Γ_2^+
icsd_025678	$CoTe_2$	58	58.397	0.00	Γ_2^+
icsd_155832	CrO_2	58	58.398	0.00	Γ_3^+
icsd_041726	$CrSb_2$	58	58.398	0.00	Γ_3^+
icsd_026756	FeS_2	58	58.397	0.00	Γ_2^+
icsd_025679	$FeTe_2$	58	58.397	0.00	Γ_2^+
icsd_048007	LiO_2Ru	58	58.398	0.00	Γ_4^+
icsd_027092	BrCrO	59	59.409	0.90	Γ_2^+
icsd_069659	BrCrS	59	59.410	0.65	Γ_4^+
icsd_010419	BrOTi	59	59.409	2.10	Γ_2^+
icsd_027010	BrOV	59	59.410	1.37	Γ_3^+
icsd_004086	ClCrO	59	59.409	1.48	Γ_2^+
icsd_261526	ClLiNTi	59	59.410	0.00	Γ_3^+
icsd_001981	ClOV	59	59.410	1.58	Γ_3^+
icsd_004202	Cu_2MgO_3	59	59.409	0.59	Γ_2^+
icsd_095957	Cu_2O_3Sr	59	59.409	0.00	Γ_2^+
icsd_088639	LiO_5V_2	59	59.409	0.35	Γ_2^+
icsd_059345	NaO_5V_2	59	59.409	0.47	Γ_2^+
icsd_185887	CrO_2	60	60.424	0.00	Γ_4^+
icsd_009496	AsMn	62	62.448	0.00	Γ_4^+
icsd_603579	BCo_2Fe	62	62.447	0.00	Γ_3^+
icsd_044339	BCo_3	62	62.446	0.00	Γ_2^+
icsd_030449	BFe	62	62.447	0.00	Γ_3^+
icsd_260757	BFe_3	62	62.446	0.00	Γ_2^+
icsd_238293	$BiMnO_3$	62	62.446	0.18	Γ_2^+
icsd_092330	$CaFeO_3$	62	62.446	0.00	Γ_2^+
icsd_670820	CAl_2Fe	62	62.447	0.00	Γ_3^+
icsd_237732	CaO_3Os	62	62.446	0.00	Γ_2^+
icsd_164775	CaO_3Rh	62	62.447	0.03	Γ_3^+
icsd_088387	CdO_3V	62	62.448	1.70	Γ_4^+
icsd_187138	CFe_2	62	62.448	0.00	Γ_4^+
icsd_670832	CFe_2Si	62	62.447	0.00	Γ_3^+
icsd_670831	$CFeNi_2$	62	62.446	0.00	Γ_2^+
icsd_623795	CoHfSi	62	62.447	0.00	Γ_3^+
icsd_601849	CoLuSi	62	62.446	0.00	Γ_2^+
icsd_049727	CoNbP	62	62.446	0.00	Γ_2^+
icsd_165256	CoNiSi	62	62.448	0.00	Γ_4^+
icsd_043249	CoP	62	62.448	0.00	Γ_4^+
icsd_624621	CoPSc	62	62.446	0.00	Γ_2^+
icsd_624636	CoPTa	62	62.446	0.00	Γ_2^+
icsd_624662	CoPW	62	62.447	0.00	Γ_3^+
icsd_066279	$CrGaSe_3$	62	62.448	0.87	Γ_4^+
icsd_014192	$CrLaOS_2$	62	62.446	1.14	Γ_2^+
icsd_626440	CrNiP	62	62.448	0.00	Γ_4^+
icsd_196498	CrPTa	62	62.448	0.00	Γ_4^+
icsd_074601	CrS_3Sb	62	62.447	0.88	Γ_3^+
icsd_084866	$CrSbSe_3$	62	62.446	0.50	Γ_2^+
icsd_000498	CuO_3Se	62	62.446	1.60	Γ_2^+
icsd_029338	CuO_3Te	62	62.448	1.48	Γ_4^+
icsd_633291	Fe_3S	62	62.448	0.00	Γ_4^+
icsd_246547	IrMnSi	62	62.446	0.00	Γ_2^+
icsd_641017	IrSiTi	62	62.447	0.00	Γ_3^+
icsd_016280	$LaMnO_3$	62	62.447	0.03	Γ_3^+
icsd_160376	$LuMnO_3$	62	62.447	0.65	Γ_3^+
icsd_191796	$LuNiO_3$	62	62.446	0.00	Γ_2^+
icsd_056617	MnO_3Y	62	62.447	0.17	Γ_3^+
icsd_041149	MnRhSi	62	62.446	0.00	Γ_2^+
icsd_093507	NiO_3Tl	62	62.446	0.00	Γ_2^+
icsd_191794	NiO_3Y	62	62.446	0.00	Γ_2^+
icsd_022303	O_2V	62	62.448	0.38	Γ_4^+
icsd_237731	O_3OsSr	62	62.447	0.00	Γ_3^+
icsd_008150	O_3TiY	62	62.446	2.09	Γ_2^+
icsd_043686	PRu_2	62	62.447	0.00	Γ_3^+

TABLE S15. Tabulated information on **ferromagnetic** materials, including the chemical formula, space group, magnetic space group, band gap and corresponding irreducible representations of crystallographic space group.

ICSD number	Chemical formula	SG NUM	BNS	Band Gap (eV)	Irrep
icsd_105931	Rh_2Sn	62	62.447	0.00	Γ_3^+
icsd_670862	Rh_3Si	62	62.446	0.00	Γ_2^+
icsd_108723	RhSiTi	62	62.448	0.00	Γ_4^+
icsd_057645	Al_2CoY	63	63.463	0.00	Γ_3^+
icsd_187136	AsFeNa	63	63.462	0.00	Γ_2^+
icsd_670104	$BaCuO_2$	63	63.463	0.08	Γ_3^+
icsd_670348	$CaMnO_3$	63	63.464	0.94	Γ_4^+
icsd_164774	CaO_3Rh	63	63.464	0.00	Γ_4^+
icsd_656056	Cs_2NiP_2	63	63.464	0.29	Γ_4^+
icsd_016217	CuO_2Sr	63	63.463	0.30	Γ_3^+
icsd_632057	$FeGe_2Lu$	63	63.462	0.00	Γ_2^+
icsd_632162	$FeGe_2Y$	63	63.462	0.00	Γ_2^+
icsd_637012	GeMnNi	63	63.462	0.00	Γ_2^+
icsd_036123	NiO_2Sr	63	63.463	0.76	Γ_3^+
icsd_043843	$Al_2B_2Ru_3$	65	65.486	0.00	Γ_3^+
icsd_020083	AlB_2Cr_2	65	65.486	0.00	Γ_3^+
icsd_020322	AlB_2Fe_2	65	65.485	0.00	Γ_2^+
icsd_025518	AlB_2Mn_2	65	65.486	0.00	Γ_4^+
icsd_082199	Br_4FeLi_2	65	65.486	3.09	Γ_3^+
icsd_033865	Br_4Li_2Mn	65	65.486	3.67	Γ_3^+
icsd_073227	Cl_4CoLi_2	65	65.486	2.59	Γ_3^+
icsd_001165	Cl_4Os	65	65.486	0.76	Γ_4^+
icsd_072872	CoO_4Re	65	65.486	0.00	Γ_4^+
icsd_035338	CoO_6Pt_3	65	65.485	0.40	Γ_2^+
icsd_174117	CuF_4K_2	65	65.486	2.17	Γ_3^+
icsd_015927	MgO_3V	65	65.485	0.00	Γ_2^+
icsd_035337	MnO_6Pt_3	65	65.486	0.39	Γ_3^+
icsd_078012	AlF_5Fe	71	71.536	4.32	Γ_3^+
icsd_613166	B_2CoMo_2	71	71.536	0.00	Γ_2^+
icsd_016776	B_2CoW_2	71	71.536	0.00	Γ_2^+
icsd_614261	B_2FeW_2	71	71.536	0.00	Γ_2^+
icsd_033704	B_4Cr_3	71	71.536	0.00	Γ_4^+
icsd_614775	B_4Mn_2Ta	71	71.536	0.00	Γ_2^+
icsd_614782	B_4Mn_2W	71	71.536	0.00	Γ_2^+
icsd_044446	B_4Mn_3	71	71.536	0.00	Γ_2^+
icsd_068795	$BaNiO_5Y_2$	71	71.536	2.09	Γ_3^+
icsd_024381	Br_2OV	71	71.536	0.57	Γ_4^+
icsd_040950	C_4CoSc_3	71	71.536	0.00	Γ_4^+
icsd_072863	C_4FeSc_3	71	71.536	0.00	Γ_2^+
icsd_016216	Ca_2CuO_3	71	71.536	0.37	Γ_2^+
icsd_024380	Cl_2OV	71	71.536	0.76	Γ_4^+
icsd_025001	$CuLi_2O_2$	71	71.536	1.36	Γ_3^+
icsd_015127	CuO_3Sr_2	71	71.536	0.20	Γ_2^+
icsd_068700	$FeLi_4N_2$	71	71.536	0.94	Γ_3^+
icsd_251018	FeO_3Sr_2	71	71.536	1.01	Γ_2^+
icsd_188992	$GaMnNi_2$	71	71.536	0.00	Γ_3^+
icsd_167658	H_2PdTi_2	71	71.536	0.00	Γ_3^+
icsd_416513	$CoPd_2Se_2$	72	72.544	0.00	Γ_4^+
icsd_416514	$CoPd_2Te_2$	72	72.543	0.00	Γ_2^+
icsd_416515	$FePd_2Se_2$	72	72.544	0.00	Γ_3^+
icsd_670341	$CaMnO_3$	74	74.559	0.22	Γ_3^+
icsd_036535	Cu_2O_2Tl	74	74.558	0.85	Γ_2^+
icsd_181038	$Cr_{0.125}Ga_{0.875}P$	81	111.255	0.00	Γ_1
icsd_090827	Cu_2FeS_4Sn	81	3.3	0.65	$\Gamma_3\Gamma_4$
icsd_052961	$CoGa_2S_4$	82	82.39	1.80	Γ_1
icsd_152909	Ga_2MnS_4	82	82.39	1.71	Γ_1
icsd_000415	Ga_2MnSe_4	82	82.39	1.54	Γ_1
icsd_018307	O_5SV	85	85.59	2.18	Γ_1^+
icsd_611737	Au_4Cr	87	12.62	0.00	$\Gamma_3^+\Gamma_4^+$
icsd_107998	Au_4Mn	87	87.75	0.00	Γ_1^+
icsd_612460	Au_4V	87	87.75	0.00	Γ_1^+
icsd_171987	Ba_2CaO_6Re	87	12.62	0.00	$\Gamma_3^+\Gamma_4^+$
icsd_191960	Ba_2CuO_6Os	87	12.62	0.10	$\Gamma_3^+\Gamma_4^+$
icsd_088703	Ba_2CuO_6Te	87	87.75	0.76	Γ_1^+
icsd_072813	Ba_2CuO_6W	87	87.75	1.39	Γ_1^+

TABLE S16. Tabulated information on **ferromagnetic** materials, including the chemical formula, space group, magnetic space group, band gap and corresponding irreducible representations of crystallographic space group.

ICSD number	Chemical formula	SG NUM	BNS	Band Gap (eV)	Irrep
icsd_095518	Ba_2FeO_6W	87	12.62	1.30	$\Gamma_3^+\Gamma_4^+$
icsd_192904	Ca_2MnO_6Ti	87	12.62	1.28	$\Gamma_3^+\Gamma_4^+$
icsd_262352	$Co_{0.5}O_3Re_{0.5}Sr$	87	12.62	0.00	$\Gamma_3^+\Gamma_4^+$
icsd_153544	$CoMoO_6Sr_2$	87	12.62	1.30	$\Gamma_3^+\Gamma_4^+$
icsd_192327	$CoNbO_6Sr_2$	87	12.62	0.60	$\Gamma_3^+\Gamma_4^+$
icsd_173488	CoO_6ReSr_2	87	12.62	0.00	$\Gamma_3^+\Gamma_4^+$
icsd_190593	CoO_6Sr_2W	87	12.62	2.12	$\Gamma_3^+\Gamma_4^+$
icsd_186038	$CuMoO_6Sr_2$	87	87.75	1.46	Γ_1^+
icsd_033573	CuO_6Sr_2Te	87	87.75	1.54	Γ_1^+
icsd_033571	CuO_6Sr_2W	87	87.75	1.74	Γ_1^+
icsd_150702	FeO_6ReSr_2	87	12.62	0.00	$\Gamma_3^+\Gamma_4^+$
icsd_078677	FeO_6Sr_2W	87	12.62	0.00	$\Gamma_3^+\Gamma_4^+$
icsd_067826	$IrNa_4O_4$	87	87.75	0.74	Γ_1^+
icsd_250818	$IrNiO_6Sr_2$	87	12.62	0.25	$\Gamma_3^+\Gamma_4^+$
icsd_194696	MgO_6OsSr_2	87	12.62	0.00	$\Gamma_3^+\Gamma_4^+$
icsd_182569	MgO_6ReSr_2	87	87.75	0.00	Γ_1^+
icsd_187669	$MnMoO_6Sr_2$	87	12.62	0.81	$\Gamma_3^+\Gamma_4^+$
icsd_098191	$MoNiO_6Sr_2$	87	12.62	2.12	$\Gamma_3^+\Gamma_4^+$
icsd_152440	NiO_6OsSr_2	87	12.62	0.00	$\Gamma_3^+\Gamma_4^+$
icsd_173487	NiO_6ReSr_2	87	87.75	0.00	Γ_1^+
icsd_009294	NiO_6Sr_2W	87	12.62	2.96	$\Gamma_3^+\Gamma_4^+$
icsd_173489	O_6ReSr_2Zn	87	87.75	0.00	Γ_1^+
icsd_066404	$BaCuFeLuO_5$	99	35.167	0.00	Γ_5
icsd_157833	$BiCoO_3$	99	99.167	0.68	Γ_4
icsd_188466	$BiFeO_3$	99	35.167	0.00	Γ_5
icsd_081589	$H_4Cl_2CuO_4Pb_2$	99	99.167	2.06	Γ_4
icsd_152276	O_3PbV	99	99.167	1.32	Γ_4
icsd_042373	$CoGe_3La$	107	107.231	0.00	Γ_4
icsd_059908	$FeGe_3La$	107	107.231	0.00	Γ_4
icsd_039351	MnO_6SbSr_2	107	107.231	0.09	Γ_4
icsd_631817	$FeGa_2Se_4$	111	111.255	0.52	Γ_4
icsd_181054	$Cd_{0.5}Cr_{0.5}Te$	115	25.59	0.00	Γ_5
icsd_181037	$Cr_{0.5}Ga_{0.5}P$	115	115.287	0.00	Γ_3
icsd_150822	FeS_2Tl	119	119.319	0.00	Γ_3
icsd_633509	$FeSe_2Tl$	119	119.319	0.00	Γ_3
icsd_087983	$KMnTe_2$	119	119.319	0.00	Γ_3
icsd_050819	$MnRbSe_2$	119	119.319	0.00	Γ_3
icsd_087984	$MnRbTe_2$	119	119.319	0.00	Γ_3
icsd_042534	Ag_2FeS_4Sn	121	23.51	0.03	Γ_5
icsd_608538	Al_2MnTe_4	121	42.221	0.88	Γ_5
icsd_016809	BFe_2	121	23.51	0.00	Γ_5
icsd_099293	$CoCu_2GeS_4$	121	121.331	0.70	Γ_4
icsd_099292	$CoCu_2S_4Si$	121	23.51	1.11	Γ_5
icsd_099294	$CoCu_2S_4Sn$	121	121.331	0.71	Γ_4
icsd_099296	$CoCu_2Se_4Sn$	121	121.331	0.19	Γ_4
icsd_108934	CrK_3O_4	121	42.221	0.89	Γ_5
icsd_047165	Cu_2FeGeS_4	121	23.51	1.02	Γ_5
icsd_627313	$Cu_2FeGeSe_4$	121	42.221	0.44	Γ_5
icsd_026721	Cu_2FeS_4Sn	121	42.221	0.78	Γ_5
icsd_627368	Cu_2FeSe_4Si	121	23.51	0.98	Γ_5
icsd_085126	Cu_2FeSe_4Sn	121	23.51	0.23	Γ_5
icsd_042489	Cu_2MnS_4Sn	121	121.331	0.72	Γ_4
icsd_155904	Cu_2MnSe_4Sn	121	121.331	0.12	Γ_4
icsd_659100	Ga_2MnSe_4	121	42.221	0.42	Γ_5
icsd_172506	$GeMnTe_4Tl_2$	121	121.331	0.13	Γ_4
icsd_639984	In_2MnTe_4	121	42.221	0.47	Γ_5
icsd_108935	K_3MnO_4	121	42.221	1.86	Γ_5
icsd_172507	$MnSnTe_4Tl_2$	121	121.331	0.26	Γ_4
icsd_107862	$AlNi_3$	123	65.486	0.00	Γ_5^+
icsd_169074	As_2BaOTi_2	123	65.486	0.00	Γ_5^+
icsd_246455	$Ba_{0.5}La_{0.5}MnO_3$	123	47.252	0.00	Γ_5^+
icsd_075730	$Ba_2Ca_2Cu_3HgO_8$	123	123.345	0.00	Γ_3^+
icsd_074163	$Ba_2Cu_2O_7TlY$	123	65.486	0.00	Γ_5^+
icsd_075720	Ba_2CuHgO_4	123	123.345	0.00	Γ_3^+
icsd_430063	$BaBi_2OTi_2$	123	47.252	0.00	Γ_5^+

TABLE S17. Tabulated information on **ferromagnetic** materials, including the chemical formula, space group, magnetic space group, band gap and corresponding irreducible representations of crystallographic space group.

ICSD number	Chemical formula	SG NUM	BNS	Band Gap (eV)	Irrep
icsd_028918	$BaFeO_3$	123	123.345	0.00	Γ_3^+
icsd_150703	$BaLaMn_2O_6$	123	47.252	0.00	Γ_5^+
icsd_237789	$BaOSb_2Ti_2$	123	47.252	0.00	Γ_5^+
icsd_088033	$BrCuLaNb_2O_7$	123	47.252	0.03	Γ_5^+
icsd_051262	$Ca_2ClCuNb_3O_{10}$	123	47.252	0.00	Γ_5^+
icsd_075868	$CaCuO_2$	123	123.345	0.00	Γ_3^+
icsd_173438	$CaFeO_2$	123	65.486	0.00	Γ_5^+
icsd_088032	$ClCuLaNb_2O_7$	123	47.252	0.76	Γ_5^+
icsd_051261	$ClCuLaO_7Ta_2$	123	47.252	0.29	Γ_5^+
icsd_157788	Co_2GaNi	123	65.486	0.00	Γ_5^+
icsd_623081	$CoGa_4Hf$	123	65.486	0.00	Γ_5^+
icsd_623236	$CoGa_5Y$	123	123.345	0.00	Γ_3^+
icsd_623111	$CoGa_8Lu_2$	123	65.486	0.00	Γ_5^+
icsd_623237	$CoGa_8Y_2$	123	123.345	0.00	Γ_3^+
icsd_150261	$CoIn_5La$	123	47.252	0.00	Γ_5^+
icsd_623947	$CoIn_5Y$	123	47.252	0.00	Γ_5^+
icsd_623948	$CoIn_8Y_2$	123	47.252	0.00	Γ_5^+
icsd_412978	$CoNa_5O_2S$	123	47.252	1.16	Γ_5^+
icsd_027690	CrF_3K	123	47.252	0.00	Γ_5^+
icsd_069675	Cs_2F_5Mn	123	123.345	1.56	Γ_3^+
icsd_027689	CuF_3K	123	65.486	1.55	Γ_5^+
icsd_109293	CuF_3Rb	123	65.486	1.60	Γ_5^+
icsd_043457	CuF_3Tl	123	65.486	0.76	Γ_5^+
icsd_021072	F_4FeRb	123	47.252	2.13	Γ_5^+
icsd_082218	F_5MnRb_2	123	123.345	1.47	Γ_3^+
icsd_186722	Fe_2GaMn	123	123.345	0.00	Γ_3^+
icsd_600147	$FeGa_8Lu_2$	123	47.252	0.00	Γ_5^+
icsd_173434	FeO_2Sr	123	65.486	0.00	Γ_5^+
icsd_184861	FeO_3Sr	123	123.347	0.00	Γ_1^-
icsd_053543	$FeSe$	123	47.252	0.00	Γ_5^+
icsd_047123	$LaNiO_2$	123	123.345	0.00	Γ_3^+
icsd_187255	$MgNi$	123	123.345	0.00	Γ_3^+
icsd_076202	$MnRh_2Sb$	123	47.252	0.00	Γ_5^+
icsd_412972	Na_5NiO_2S	123	123.345	1.47	Γ_3^+
icsd_028837	OPd	123	47.252	0.00	Γ_5^+
icsd_623784	$CoHf_4P$	124	124.357	0.00	Γ_3^+
icsd_632255	$FeHf_4P$	124	66.496	0.00	Γ_5^+
icsd_632795	$FeNb_4P$	124	66.496	0.00	Γ_5^+
icsd_053511	$FeNb_4Si$	124	66.496	0.00	Γ_5^+
icsd_613529	B_2CrNb_2	127	65.486	0.00	Γ_5^+
icsd_613557	B_2CrTa_2	127	65.486	0.00	Γ_5^+
icsd_044449	B_2MnW_2	127	55.358	0.00	Γ_5^+
icsd_615683	B_4W	127	127.393	0.00	Γ_3^+
icsd_249632	Ga_5Mn_2	127	65.486	0.00	Γ_5^+
icsd_104026	Ga_5V_2	127	55.358	0.00	Γ_5^+
icsd_245749	Cl_6K_2Nb	128	58.398	0.06	Γ_5^+
icsd_042750	$AlGeMn$	129	129.417	0.00	Γ_3^+
icsd_262356	$As_2Co_2O_6Sc_2Sr_4$	129	67.506	0.00	Γ_5^+
icsd_610777	As_2LaRh_2	129	129.417	0.00	Γ_3^+
icsd_167818	$AsCoLaO$	129	129.417	0.00	Γ_3^+
icsd_107932	$AsCoLi$	129	129.417	0.00	Γ_3^+
icsd_062598	C_2CoSc	129	129.417	0.00	Γ_3^+
icsd_617820	C_2FeSc	129	59.410	0.00	Γ_5^+
icsd_085283	$CBNiY$	129	59.410	0.00	Γ_5^+
icsd_090122	$ClCoO_3Sr_2$	129	67.506	0.00	Γ_5^+
icsd_050988	$ClKMoO_5P$	129	129.417	1.36	Γ_3^+
icsd_094745	$ClMnO_3Sr_2$	129	129.417	0.00	Γ_3^+
icsd_050989	$ClMoO_5PRb$	129	129.417	1.30	Γ_3^+
icsd_237581	$ClNiO_3Sr_2$	129	67.506	0.00	Γ_5^+
icsd_418853	$CoGeMg$	129	129.417	0.00	Γ_3^+
icsd_015770	$CoKO_2$	129	129.417	0.73	Γ_3^+
icsd_080203	$CoLaOP$	129	67.506	0.00	Γ_5^+
icsd_248374	$CoMnSb$	129	67.506	0.00	Γ_5^+
icsd_624599	$CoPPd$	129	67.506	0.00	Γ_5^+
icsd_162902	$CoSe$	129	59.410	0.00	Γ_5^+

TABLE S18. Tabulated information on **ferromagnetic** materials, including the chemical formula, space group, magnetic space group, band gap and corresponding irreducible representations of crystallographic space group.

ICSD number	Chemical formula	SG NUM	BNS	Band Gap (eV)	Irrep
icsd_191258	CrN_3Nb	129	129.417	0.00	Γ_3^+
icsd_091199	$CuMnO_3SSr_2$	129	129.417	0.00	Γ_3^+
icsd_194319	FeNSe	129	67.506	0.00	Γ_5^+
icsd_107617	GeLaTi	129	129.417	0.00	Γ_3^+
icsd_086777	$GeLi_2O_5V$	129	129.417	2.33	Γ_3^+
icsd_085904	GeTiY	129	59.410	0.00	Γ_5^+
icsd_059359	Li_2O_5SiV	129	129.417	2.59	Γ_3^+
icsd_088208	LuSiTi	129	59.410	0.00	Γ_5^+
icsd_162903	NiSe	129	129.417	0.00	Γ_3^+
icsd_088113	SiTiY	129	67.506	0.00	Γ_5^+
icsd_069044	CaNNi	131	66.496	0.00	Γ_5^+
icsd_061691	CCoLu	131	47.252	0.00	Γ_5^+
icsd_061684	CCoY	131	47.252	0.00	Γ_5^+
icsd_187715	NOs	131	131.441	0.00	Γ_3^+
icsd_187709	NTc	131	66.496	0.00	Γ_5^+
icsd_072387	$CoLiN_2Sr_2$	136	136.501	0.32	Γ_3^+
icsd_108964	CoO_6Sb_2	136	65.486	0.93	Γ_5^+
icsd_173874	Cr_2O_6Re	136	136.501	0.00	Γ_3^+
icsd_009423	CrO_2	136	136.501	0.00	Γ_3^+
icsd_130032	Cu_2Hf_2In	136	136.501	0.00	Γ_3^+
icsd_130034	Cu_2InZr_2	136	136.501	0.00	Γ_3^+
icsd_290252	F_6Li_2V	136	136.501	2.21	Γ_3^+
icsd_035382	F_6LiV_2	136	136.501	0.00	Γ_3^+
icsd_068525	Fe_4P_2Sc	136	58.398	0.00	Γ_5^+
icsd_633122	Fe_4P_2Zr	136	58.398	0.00	Γ_5^+
icsd_087172	Fe_4Si_2Zr	136	58.398	0.00	Γ_5^+
icsd_040344	FeO_6Sb_2	136	58.398	0.06	Γ_5^+
icsd_189495	Ni_4P_2Y	136	38.190	0.00	Γ_3^+
icsd_080802	NiO_6Sb_2	136	136.501	1.28	Γ_3^+
icsd_061198	NiO_6Ta_2	136	136.501	2.91	Γ_3^+
icsd_076024	O_2Ta	136	136.501	0.00	Γ_3^+
icsd_001504	O_2V	136	136.501	0.74	Γ_3^+
icsd_238076	$Ag_2Ba_2CoO_2Se_2$	139	71.536	0.50	Γ_5^+
icsd_016254	$AgCs_2F_4$	139	69.524	0.00	Γ_5^+
icsd_609234	Al_2Ru	139	139.537	0.00	Γ_3^+
icsd_085659	$As_2Ba_2MnO_2Zn_2$	139	69.524	0.00	Γ_5^+
icsd_610072	As_2Co_2K	139	139.537	0.00	Γ_3^+
icsd_610297	As_2CsRu_2	139	139.537	0.00	Γ_3^+
icsd_167013	$As_2F_2OSr_2Ti_2$	139	71.536	0.00	Γ_5^+
icsd_604549	B_2Fe_2Lu	139	139.537	0.00	Γ_3^+
icsd_614264	B_2Fe_2Y	139	139.537	0.00	Γ_3^+
icsd_054042	$B_2La_3N_3Ni_2$	139	139.537	0.00	Γ_3^+
icsd_261352	$Ba_2CoCu_2O_2S_2$	139	69.524	0.80	Γ_5^+
icsd_021057	Ba_2CoF_6	139	69.524	3.39	Γ_5^+
icsd_033569	Ba_2CuO_6W	139	139.537	1.60	Γ_3^+
icsd_021056	Ba_2F_6Ni	139	139.537	3.94	Γ_3^+
icsd_155174	Ba_2FeO_6Re	139	139.537	0.00	Γ_3^+
icsd_420975	$BaCo_2Ge_2$	139	139.537	0.00	Γ_3^+
icsd_001028	$Br_2Ca_2CuO_2$	139	139.537	0.00	Γ_3^+
icsd_059698	$Br_2CoO_2Sr_2$	139	69.524	1.11	Γ_5^+
icsd_008174	Br_4MnRb_2	139	69.524	2.58	Γ_5^+
icsd_001027	$Ca_2Cl_2CuO_2$	139	139.537	0.00	Γ_3^+
icsd_425467	$CaFe_2Si_2$	139	71.536	0.00	Γ_5^+
icsd_059697	$Cl_2CoO_2Sr_2$	139	69.524	1.04	Γ_5^+
icsd_004087	$Cl_2CuO_2Sr_2$	139	139.537	0.00	Γ_3^+
icsd_041571	Cl_4CrCs_2	139	71.536	0.00	Γ_5^+
icsd_009857	Cl_4CrRb_2	139	139.537	0.00	Γ_3^+
icsd_001139	Cl_4MnRb_2	139	71.536	3.35	Γ_5^+
icsd_245748	Cl_6NbRb_2	139	69.524	0.00	Γ_5^+
icsd_081750	Co_2Ge_2La	139	139.537	0.00	Γ_3^+
icsd_623956	Co_2KS_2	139	71.536	0.00	Γ_5^+
icsd_067370	Co_2KSe_2	139	71.536	0.00	Γ_5^+
icsd_624795	Co_2RbS_2	139	69.524	0.00	Γ_5^+
icsd_624798	Co_2RbSe_2	139	69.524	0.00	Γ_5^+
icsd_067362	Co_2Se_2Tl	139	69.524	0.00	Γ_5^+

TABLE S19. Tabulated information on **ferromagnetic** materials, including the chemical formula, space group, magnetic space group, band gap and corresponding irreducible representations of crystallographic space group.

ICSD number	Chemical formula	SG NUM	BNS	Band Gap (eV)	Irrep
icsd_074889	$CoCsK_2O_2$	139	69.524	1.93	Γ_5^+
icsd_033522	CoF_4K_2	139	69.524	3.78	Γ_5^+
icsd_069683	CoF_4Rb_2	139	69.524	3.84	Γ_5^+
icsd_670534	$CoFeLa_2O_6$	139	139.537	1.81	Γ_3^+
icsd_191364	$CoHfO_6Sr_2$	139	139.537	0.00	Γ_3^+
icsd_191362	$CoLaO_6Sr_2$	139	71.536	0.62	Γ_5^+
icsd_053059	CoO	139	71.536	1.85	Γ_5^+
icsd_246483	CoO_4Sr_2	139	71.536	0.00	Γ_5^+
icsd_405782	CoO_6Pb_2Te	139	71.536	2.06	Γ_5^+
icsd_191361	CoO_6Sr_2Y	139	71.536	0.32	Γ_5^+
icsd_191363	CoO_6Sr_2Zr	139	71.536	0.23	Γ_5^+
icsd_075384	CrF_6Nb	139	69.524	0.00	Γ_5^+
icsd_191358	$CrHfO_6Sr_2$	139	71.536	0.00	Γ_5^+
icsd_191357	CrO_6Sr_2Zr	139	71.536	0.00	Γ_5^+
icsd_065259	Cs_2CuF_6	139	69.524	0.31	Γ_5^+
icsd_039535	Cs_2CuO_2	139	139.537	0.00	Γ_3^+
icsd_091036	Cs_2F_6KMn	139	139.537	1.75	Γ_3^+
icsd_423923	Cs_2NiO_2	139	69.524	2.31	Γ_5^+
icsd_084734	$Cu_2MnO_2S_2Sr_2$	139	69.524	0.00	Γ_5^+
icsd_088424	$Cu_2NiO_2S_2Sr_2$	139	69.524	0.11	Γ_5^+
icsd_088423	$Cu_3O_2S_2Sr_2$	139	139.537	0.00	Γ_3^+
icsd_015372	CuF_4K_2	139	69.524	2.09	Γ_5^+
icsd_055710	$CuI_2O_2Sr_2$	139	71.536	0.00	Γ_5^+
icsd_039475	$CuIn_2O_4$	139	139.537	0.00	Γ_3^+
icsd_041643	$CuLa_2O_4$	139	139.537	0.00	Γ_3^+
icsd_167014	$F_2OSb_2Sr_2Ti_2$	139	71.536	0.00	Γ_5^+
icsd_023183	F_4K_2Mn	139	69.524	2.77	Γ_5^+
icsd_015576	F_4K_2Ni	139	139.537	3.85	Γ_3^+
icsd_023949	F_4Nb	139	139.537	0.00	Γ_3^+
icsd_069682	F_4NiRb_2	139	139.537	3.89	Γ_3^+
icsd_009708	$F_6MnNaRb_2$	139	139.537	1.65	Γ_3^+
icsd_081747	Fe_2Ge_2La	139	139.537	0.00	Γ_3^+
icsd_081745	Fe_2Ge_2Y	139	69.524	0.00	Γ_5^+
icsd_186572	Fe_2KS_2	139	69.524	0.00	Γ_5^+
icsd_186573	Fe_2KSe_2	139	71.536	0.00	Γ_5^+
icsd_186574	Fe_2KTe_2	139	71.536	0.00	Γ_5^+
icsd_632475	Fe_2LuSi_2	139	71.536	0.00	Γ_5^+
icsd_633338	Fe_2S_2Tl	139	139.537	0.00	Γ_3^+
icsd_053544	Fe_2Se_2Tl	139	139.537	0.00	Γ_3^+
icsd_191366	$FeHfO_6Sr_2$	139	69.524	0.00	Γ_5^+
icsd_670535	$FeIrLa_2O_6$	139	139.537	0.46	Γ_3^+
icsd_069849	FeO_4Sr_2	139	71.536	0.00	Γ_5^+
icsd_191365	FeO_6Sr_2Zr	139	139.537	0.59	Γ_3^+
icsd_670137	Ga_3Mo	139	139.537	0.00	Γ_3^+
icsd_634592	Ga_4LuTi_2	139	139.537	0.00	Γ_3^+
icsd_635352	Ga_4ScTi_2	139	139.537	0.00	Γ_3^+
icsd_103999	Ga_4Ti_2Y	139	139.537	0.00	Γ_3^+
icsd_635567	Ga_4Ti_2Zr	139	139.537	0.00	Γ_3^+
icsd_153292	$GaMnNi_2$	139	139.537	0.00	Γ_3^+
icsd_107040	Ge_2LuMn_2	139	71.536	0.00	Γ_5^+
icsd_053715	Ge_2Mn_2Y	139	71.536	0.00	Γ_5^+
icsd_090234	GeTiY	139	69.524	0.00	Γ_5^+
icsd_168287	Hf_2Tl	139	71.536	0.00	Γ_5^+
icsd_191630	$HfLa_2NiO_6$	139	71.536	1.64	Γ_5^+
icsd_191360	HfO_6Sr_2V	139	71.536	0.94	Γ_5^+
icsd_072191	I_2La	139	139.537	0.00	Γ_3^+
icsd_021069	K_2NiO_2	139	71.536	2.37	Γ_5^+
icsd_181385	$La_2Mn_2O_3Se_2$	139	69.524	1.79	Γ_5^+
icsd_001179	La_2NiO_4	139	69.524	0.88	Γ_5^+
icsd_191628	La_2NiO_6Ti	139	71.536	2.32	Γ_5^+
icsd_191629	La_2NiO_6Zr	139	71.536	1.55	Γ_5^+
icsd_169470	La_2O_6ReV	139	139.537	0.14	Γ_3^+
icsd_090197	$LuRu_2Si_2$	139	69.524	0.00	Γ_5^+
icsd_098525	MgO_6ReSr_2	139	139.537	0.00	Γ_3^+
icsd_082937	Mn_2Si_2Y	139	71.536	0.00	Γ_5^+

TABLE S20. Tabulated information on **ferromagnetic** materials, including the chemical formula, space group, magnetic space group, band gap and corresponding irreducible representations of crystallographic space group.

ICSD number	Chemical formula	SG NUM	BNS	Band Gap (eV)	Irrep
icsd_106932	MnN	139	69.524	0.00	Γ_5^+
icsd_026560	MnO_4Sr_2	139	71.536	0.00	Γ_5^+
icsd_152123	MoO_4Sr_2	139	69.524	0.00	Γ_5^+
icsd_073209	Na_2NiO_2Rb	139	139.537	1.52	Γ_3^+
icsd_069648	$Na_2OSb_2Ti_2$	139	69.524	0.00	Γ_5^+
icsd_066277	NiO_2Rb_2	139	69.524	2.45	Γ_5^+
icsd_239358	O_4RhSr_2	139	139.537	0.00	Γ_3^+
icsd_033802	O_4RuSr_2	139	139.537	0.00	Γ_3^+
icsd_236760	O_4Sr_2Tc	139	71.536	0.00	Γ_5^+
icsd_069000	O_4Sr_2V	139	139.537	0.00	Γ_3^+
icsd_191359	O_6Sr_2VZr	139	71.536	0.91	Γ_5^+
icsd_042530	BFe_2	140	69.524	0.00	Γ_5^+
icsd_102672	$CoSn_2$	140	69.524	0.00	Γ_5^+
icsd_042519	$FeGe_2$	140	140.547	0.00	Γ_3^+
icsd_186636	$FeSb_2$	140	69.524	0.00	Γ_5^+
icsd_024570	$FeSn_2$	140	69.524	0.00	Γ_5^+
icsd_024571	$MnSn_2$	140	72.544	0.00	Γ_5^+
icsd_086940	O_3RuSr	140	140.547	0.00	Γ_3^+
icsd_031149	$Fe_2Li_2O_4$	141	70.530	0.59	Γ_5^+
icsd_162264	$BiFeO_3$	146	1.1	0.21	$\Gamma_2\Gamma_3$
icsd_193740	$H_4As_3MnNS_6$	146	1.1	1.97	$\Gamma_2\Gamma_3$
icsd_091527	$KNiO_9P_3$	146	146.10	4.55	Γ_1
icsd_408193	$Ag_2BaMnO_8V_2$	147	2.4	2.43	$\Gamma_2^+\Gamma_3^+$
icsd_194590	$Ag_2FeKO_8V_2$	147	2.4	2.02	$\Gamma_2^+\Gamma_3^+$
icsd_194588	$Ag_2FeO_8RbV_2$	147	2.4	1.99	$\Gamma_2^+\Gamma_3^+$
icsd_429825	$BaLi_2MnO_8V_2$	147	2.4	2.96	$\Gamma_2^+\Gamma_3^+$
icsd_051015	CoO_8Re_2	147	2.4	2.20	$\Gamma_2^+\Gamma_3^+$
icsd_164948	CrO_6TeY	147	15.85	1.07	$\Gamma_2^+\Gamma_3^+$
icsd_245667	$CsFeO_8S_2$	147	2.4	1.53	$\Gamma_2^+\Gamma_3^+$
icsd_073736	CsO_8S_2V	147	2.4	2.20	$\Gamma_2^+\Gamma_3^+$
icsd_245666	$FeMo_2O_8Rb$	147	2.4	2.54	$\Gamma_2^+\Gamma_3^+$
icsd_051014	MnO_8Re_2	147	2.4	3.59	$\Gamma_2^+\Gamma_3^+$
icsd_051016	NiO_8Re_2	147	147.13	2.47	Γ_1^+
icsd_260062	$As_2BaCo_2O_8$	148	148.17	3.00	Γ_1^+
icsd_671511	$AsInNi_3$	148	2.4	0.00	$\Gamma_2^+\Gamma_3^+$
icsd_237739	Au_5MnY_3	148	148.17	0.00	Γ_1^+
icsd_079165	B_2MnO_6Sn	148	148.17	2.91	Γ_1^+
icsd_174290	Ba_2BiIrO_6	148	2.4	0.20	$\Gamma_2^+\Gamma_3^+$
icsd_152678	Ba_2IrLaO_6	148	2.4	0.49	$\Gamma_2^+\Gamma_3^+$
icsd_155549	Ba_2LaO_6Ru	148	148.17	1.29	Γ_1^+
icsd_419467	$Ba_6N_6OOs_2$	148	2.4	0.00	$\Gamma_2^+\Gamma_3^+$
icsd_240981	BaF_6Ir	148	148.17	1.17	Γ_1^+
icsd_062157	$BaMo_6S_8$	148	2.4	0.00	$\Gamma_2^+\Gamma_3^+$
icsd_076421	Br_3Fe	148	2.4	0.75	$\Gamma_2^+\Gamma_3^+$
icsd_039242	Br_3Ti	148	2.4	2.22	$\Gamma_2^+\Gamma_3^+$
icsd_010343	$CaCrF_6$	148	2.4	0.96	$\Gamma_2^+\Gamma_3^+$
icsd_042160	CaF_6Rh	148	2.4	0.48	$\Gamma_2^+\Gamma_3^+$
icsd_670349	$CaMnO_3$	148	148.17	1.64	Γ_1^+
icsd_033288	Cl_2CoO_8	148	148.17	3.64	Γ_1^+
icsd_033289	Cl_2NiO_8	148	2.4	3.18	$\Gamma_2^+\Gamma_3^+$
icsd_022081	Cl_3Cr	148	148.17	2.23	Γ_1^+
icsd_002552	Cl_3MnNa	148	148.17	4.16	Γ_1^+
icsd_038237	Cl_3V	148	2.4	1.75	$\Gamma_2^+\Gamma_3^+$
icsd_425145	Cl_6Re	148	148.17	0.00	Γ_1^+
icsd_025014	CoF_6Sn	148	148.17	3.67	Γ_1^+
icsd_016548	CoO_3Ti	148	2.4	3.07	$\Gamma_2^+\Gamma_3^+$
icsd_169192	CoO_6Pb_2Te	148	148.17	1.19	Γ_1^+
icsd_079268	$Cr_2Ge_2Te_6$	148	148.17	0.01	Γ_1^+
icsd_071020	$Cr_2Si_2Te_6$	148	148.17	0.09	Γ_1^+
icsd_010347	CrF_6Hg	148	148.17	0.52	Γ_1^+
icsd_418672	CrF_6K	148	2.4	0.93	$\Gamma_2^+\Gamma_3^+$
icsd_010344	CrF_6Mg	148	2.4	0.92	$\Gamma_2^+\Gamma_3^+$
icsd_418671	CrF_6Na	148	148.17	0.95	Γ_1^+
icsd_418673	CrF_6Rb	148	2.4	0.92	$\Gamma_2^+\Gamma_3^+$
icsd_251655	CrI_3	148	148.17	0.63	Γ_1^+

TABLE S21. Tabulated information on **ferromagnetic** materials, including the chemical formula, space group, magnetic space group, band gap and corresponding irreducible representations of crystallographic space group.

ICSD number	Chemical formula	SG NUM	BNS	Band Gap (eV)	Irrep
icsd_626809	$CrSiTe_3$	148	148.17	0.06	Γ_1^+
icsd_201511	CsF_6Re	148	148.17	0.32	Γ_1^+
icsd_025016	CuF_6Sn	148	148.17	1.67	Γ_1^+
icsd_030116	CuF_6Zr	148	148.17	3.55	Γ_1^+
icsd_025011	F_6FeSn	148	2.4	3.06	$\Gamma_2^+\Gamma_3^+$
icsd_042163	F_6HgRh	148	2.4	0.40	$\Gamma_2^+\Gamma_3^+$
icsd_095777	F_6IrLi	148	148.17	0.80	Γ_1^+
icsd_027664	F_6KOs	148	148.17	1.74	Γ_1^+
icsd_165215	F_6KRh	148	2.4	0.23	$\Gamma_2^+\Gamma_3^+$
icsd_165206	F_6LiOs	148	148.17	1.64	Γ_1^+
icsd_165208	F_6LiPt	148	2.4	0.39	$\Gamma_2^+\Gamma_3^+$
icsd_095776	F_6LiRh	148	148.17	0.13	Γ_1^+
icsd_165203	F_6LiRu	148	2.4	1.98	$\Gamma_2^+\Gamma_3^+$
icsd_042159	F_6MgRh	148	2.4	0.39	$\Gamma_2^+\Gamma_3^+$
icsd_025010	F_6MnSn	148	2.4	3.29	$\Gamma_2^+\Gamma_3^+$
icsd_015108	F_6NiPb	148	2.4	1.83	$\Gamma_2^+\Gamma_3^+$
icsd_025015	F_6NiSn	148	148.17	2.99	Γ_1^+
icsd_042161	F_6RhZn	148	2.4	0.44	$\Gamma_2^+\Gamma_3^+$
icsd_063304	$FeI_{12}Y_7$	148	2.4	0.00	$\Gamma_2^+\Gamma_3^+$
icsd_639106	$HgMo_6S_8$	148	1.1	0.00	$\Gamma_2^+\Gamma_3^+$
icsd_035145	$I_{12}Zr_6$	148	2.4	0.06	$\Gamma_2^+\Gamma_3^+$
icsd_245005	$In_6O_{12}Re$	148	2.4	0.04	$\Gamma_2^+\Gamma_3^+$
icsd_061217	$IrLi_8O_6$	148	2.4	0.85	$\Gamma_2^+\Gamma_3^+$
icsd_641241	KMo_6S_8	148	148.18	0.00	Γ_1^+
icsd_059175	KO_8S_2V	148	2.4	2.33	$\Gamma_2^+\Gamma_3^+$
icsd_062156	Mo_6S_8Sr	148	148.17	0.00	Γ_1^+
icsd_262503	$C_6Ag_3KMnN_6$	149	5.15	2.50	Γ_3
icsd_201056	$C_6Au_3CoKN_6$	149	5.13	1.89	Γ_3
icsd_249724	$C_6Au_3KN_6Ni$	149	5.13	1.83	Γ_3
icsd_060313	$IKNiO_6$	149	5.13	0.16	Γ_3
icsd_150675	$CrLiS_2$	150	12.58	1.22	Γ_3
icsd_075550	FeO_8RbSe_2	150	5.15	2.18	Γ_3
icsd_169980	$HNiO_2$	156	156.51	0.00	Γ_2
icsd_050817	$LiMnSe_2$	156	8.32	0.00	Γ_3
icsd_110773	$LiMnTe_2$	156	8.34	0.00	Γ_3
icsd_050818	$MnNaSe_2$	156	8.32	0.00	Γ_3
icsd_110774	$MnNaTe_2$	156	8.32	0.00	Γ_3
icsd_182698	$H_4Ni_3O_9Si_2$	157	157.55	3.13	Γ_2
icsd_024797	$AgCrS_2$	160	8.32	0.91	Γ_3
icsd_024799	$AgCrSe_2$	160	8.32	0.00	Γ_3
icsd_605002	$AgCrTe_2$	160	8.32	0.00	Γ_3
icsd_605616	$AgNiSe_2$	160	8.32	0.00	Γ_3
icsd_605619	$AgNiTe_2$	160	8.32	0.00	Γ_3
icsd_036564	$AlMo_4S_8$	160	8.32	0.16	Γ_3
icsd_088852	$AuCrS_2$	160	8.34	0.65	Γ_3
icsd_020288	$BiFeO_3$	160	166.101	0.00	Γ_2
icsd_024796	$CrCuS_2$	160	8.34	0.59	Γ_3
icsd_024798	$CrCuSe_2$	160	8.32	0.00	Γ_3
icsd_084639	CrN_2W	160	160.67	0.00	Γ_2
icsd_201396	CrS_2Tl	160	160.67	0.00	Γ_2
icsd_626736	$CrSe_2Tl$	160	8.32	0.00	Γ_3
icsd_033995	$GaMo_4S_8$	160	8.32	0.28	Γ_3
icsd_036563	$GaMo_4Se_8$	160	8.32	0.31	Γ_3
icsd_158199	GaS_8V_4	160	8.32	0.01	Γ_3
icsd_195253	$GaSe_8V_4$	160	8.32	0.00	Γ_3
icsd_069571	$H_6F_3O_3V$	160	8.34	2.74	Γ_3
icsd_001372	$HCrO_2$	160	160.67	2.12	Γ_2
icsd_639980	In_2MnSe_4	160	160.67	0.00	Γ_2
icsd_641335	KS_2Ti	160	8.32	0.26	Γ_3
icsd_644994	NaS_2V	160	8.32	0.41	Γ_3
icsd_077990	RbS_2Ti	160	8.32	0.00	Γ_3
icsd_043410	S_2Ta	160	8.34	0.00	Γ_3
icsd_024315	Se_2Ta	160	8.34	0.00	Γ_3
icsd_187684	NiO_3Pb	161	161.71	0.00	Γ_2
icsd_080350	As_2CoO_6	162	162.77	2.74	Γ_2^+

TABLE S22. Tabulated information on **ferromagnetic** materials, including the chemical formula, space group, magnetic space group, band gap and corresponding irreducible representations of crystallographic space group.

ICSD number	Chemical formula	SG NUM	BNS	Band Gap (eV)	Irrep
icsd_080351	As_2MnO_6	162	12.62	2.18	Γ_3^+
icsd_080349	As_2NiO_6	162	12.58	2.80	Γ_3^+
icsd_187098	As_2O_6Pd	162	12.58	1.51	Γ_3^+
icsd_173552	$C_6Ag_3FeN_6$	162	12.58	1.87	Γ_3^+
icsd_043292	Cl_3Zr	162	162.77	0.00	Γ_2^+
icsd_201755	F_6Li_2Nb	162	12.62	0.10	Γ_3^+
icsd_291234	MnO_6Sb_2	162	12.62	1.35	Γ_3^+
icsd_073985	$CaCrF_6Li$	163	163.83	3.57	Γ_2^+
icsd_062035	Cl_6CrNa_3	163	15.89	2.69	Γ_3^+
icsd_043278	$AgFeTe_2$	164	164.89	0.00	Γ_2^+
icsd_609482	Al_3Tc_2	164	164.89	0.00	Γ_2^+
icsd_423734	Ba_2Ni_3	164	164.89	0.00	Γ_2^+
icsd_246280	$Ba_3CaIr_2O_9$	164	164.89	0.00	Γ_2^+
icsd_150431	$Ba_3CoNb_2O_9$	164	164.89	2.20	Γ_2^+
icsd_171479	$Ba_3MnNb_2O_9$	164	164.89	1.65	Γ_2^+
icsd_240281	$Ba_3NiO_9Ta_2$	164	12.58	3.55	Γ_3^+
icsd_429826	$BaCoNa_2O_8V_2$	164	12.58	3.08	Γ_3^+
icsd_429827	$BaFeNa_2O_8V_2$	164	12.62	2.37	Γ_3^+
icsd_429824	$BaLi_2MnO_8V_2$	164	12.58	3.43	Γ_3^+
icsd_052364	Br_2Co	164	12.58	2.30	Γ_3^+
icsd_052365	Br_2Fe	164	12.62	2.39	Γ_3^+
icsd_060250	Br_2Mn	164	164.89	3.15	Γ_2^+
icsd_026078	Br_2Ti	164	164.89	0.00	Γ_2^+
icsd_246906	Br_2V	164	12.58	2.98	Γ_3^+
icsd_064831	Cl_2Fe	164	12.62	2.97	Γ_3^+
icsd_023177	Cl_2Ti	164	164.89	0.00	Γ_2^+
icsd_015901	Cl_2V	164	12.62	3.21	Γ_3^+
icsd_052368	CoI_2	164	12.58	1.43	Γ_3^+
icsd_088722	CoO_2	164	12.58	0.98	Γ_3^+
icsd_625401	$CoTe_2$	164	12.58	0.00	Γ_3^+
icsd_626052	$CrGa_2S_4$	164	164.89	0.00	Γ_2^+
icsd_026233	$CrLiS_2$	164	12.62	1.21	Γ_3^+
icsd_626718	$CrSe_2$	164	12.62	0.00	Γ_3^+
icsd_079007	$CrTe_2Tl$	164	164.89	0.00	Γ_2^+
icsd_240956	Cs_2F_6Ir	164	12.62	1.21	Γ_3^+
icsd_072832	Cs_2F_6Nb	164	12.62	0.00	Γ_3^+
icsd_425912	Cs_2F_6Tc	164	164.89	3.11	Γ_2^+
icsd_260887	$CsFeMo_2O_8$	164	12.58	2.59	Γ_3^+
icsd_202907	$CsMo_2O_8V$	164	12.62	1.77	Γ_3^+
icsd_095779	F_6IrK_2	164	12.62	1.11	Γ_3^+
icsd_240955	F_6IrRb_2	164	12.62	1.16	Γ_3^+
icsd_001528	F_6K_2Re	164	164.89	1.63	Γ_2^+
icsd_028779	F_6K_2Rh	164	12.62	0.47	Γ_3^+
icsd_425914	F_6K_2Tc	164	164.89	3.02	Γ_2^+
icsd_425915	F_6Na_2Tc	164	164.89	3.07	Γ_2^+
icsd_072831	F_6NbRb_2	164	12.58	0.40	Γ_3^+
icsd_028780	F_6Rb_2Rh	164	12.62	0.53	Γ_3^+
icsd_425918	F_6Rb_2Tc	164	164.89	3.07	Γ_2^+
icsd_100706	$FeGa_2S_4$	164	12.58	0.65	Γ_3^+
icsd_052369	FeI_2	164	12.58	1.69	Γ_3^+
icsd_153864	$FeKMo_2O_8$	164	12.62	2.44	Γ_3^+
icsd_632443	$FeLi_2S_2$	164	12.62	1.99	Γ_3^+
icsd_245665	$FeMo_2O_8Rb$	164	12.62	2.30	Γ_3^+
icsd_059230	Ga_2NiS_4	164	12.58	0.98	Γ_3^+
icsd_088940	H_2CoO_2	164	12.58	2.89	Γ_3^+
icsd_023591	H_2MnO_2	164	164.89	1.27	Γ_2^+
icsd_028101	H_2NiO_2	164	164.89	2.90	Γ_2^+
icsd_240663	$H_6Cl_2Cu_3MgO_6$	164	164.89	2.17	Γ_2^+
icsd_162099	$H_6Cl_2Cu_3O_6Zn$	164	164.89	2.37	Γ_2^+
icsd_033673	I_2Mn	164	164.89	2.23	Γ_2^+
icsd_246907	I_2V	164	12.58	2.67	Γ_3^+
icsd_100782	$K_3O_8V_3$	164	12.62	1.69	Γ_3^+
icsd_037327	Li_2MnO_2	164	164.89	2.55	Γ_2^+
icsd_071421	Li_2NiO_2	164	164.89	3.24	Γ_2^+
icsd_200709	LiS_2Ti	164	12.58	0.00	Γ_3^+

TABLE S23. Tabulated information on **ferromagnetic** materials, including the chemical formula, space group, magnetic space group, band gap and corresponding irreducible representations of crystallographic space group.

ICSD number	Chemical formula	SG NUM	BNS	Band Gap (eV)	Irrep
icsd_016303	LiS_2V	164	12.62	0.54	Γ_3^+
icsd_044908	$LiTe_2Ti$	164	12.58	0.00	Γ_3^+
icsd_182700	N_3V_2	164	164.89	0.00	Γ_2^+
icsd_644993	NaS_2V	164	12.58	0.00	Γ_3^+
icsd_042559	$NiTe_2$	164	164.89	0.00	Γ_2^+
icsd_086519	S_2V	164	12.58	0.02	Γ_3^+
icsd_086520	Se_2V	164	12.62	0.00	Γ_3^+
icsd_603582	Te_2V	164	12.62	0.00	Γ_3^+
icsd_160574	Ag_2NiO_2	166	12.58	0.00	Γ_3^+
icsd_004149	$AgCrO_2$	166	166.101	1.40	Γ_2^+
icsd_031919	$AgFeO_2$	166	166.101	1.17	Γ_2^+
icsd_073974	$AgNiO_2$	166	12.58	0.00	Γ_3^+
icsd_670082	$AuCrO_2$	166	12.58	0.91	Γ_3^+
icsd_670084	$AuFeO_2$	166	166.101	0.36	Γ_2^+
icsd_074030	Ba_2IrO_6Sr	166	166.101	0.37	Γ_2^+
icsd_407802	Ba_2MnO_6Te	166	12.58	1.35	Γ_3^+
icsd_009457	$Ba_3Cr_2O_8$	166	166.101	0.48	Γ_2^+
icsd_010341	$BaCrF_6$	166	166.101	0.93	Γ_2^+
icsd_035396	BaF_6Ni	166	12.62	0.30	Γ_3^+
icsd_006038	BaF_6Rh	166	166.101	0.30	Γ_2^+
icsd_425966	Bi_2MnTe_4	166	166.101	0.05	Γ_2^+
icsd_020372	$BiFeO_3$	166	166.101	0.00	Γ_2^+
icsd_067500	Br_2Mn	166	166.101	3.21	Γ_2^+
icsd_022106	Br_2Ni	166	12.58	1.96	Γ_3^+
icsd_023354	BrLa	166	12.58	0.00	Γ_3^+
icsd_074680	$Cl_{12}OsS_2$	166	12.58	0.81	Γ_3^+
icsd_015939	Cl_2Co	166	12.62	2.93	Γ_3^+
icsd_004059	Cl_2Fe	166	12.62	3.00	Γ_3^+
icsd_033752	Cl_2Mn	166	166.101	3.80	Γ_2^+
icsd_014208	Cl_2Ni	166	12.58	2.67	Γ_3^+
icsd_024410	ClLa	166	12.58	0.00	Γ_3^+
icsd_001004	ClSc	166	166.101	0.00	Γ_2^+
icsd_170135	$CMnN_2$	166	166.101	1.93	Γ_2^+
icsd_416314	$Co_{1.5}SSn$	166	12.58	0.00	Γ_3^+
icsd_005436	$Co_3In_2S_2$	166	12.58	0.00	Γ_3^+
icsd_005437	Co_3InS_2Sn	166	166.101	0.00	Γ_2^+
icsd_005435	$Co_3S_2Sn_2$	166	12.62	0.00	Γ_3^+
icsd_027803	$CoCuO_2$	166	12.58	0.72	Γ_3^+
icsd_670109	$CoCuO_2$	166	12.62	0.18	Γ_3^+
icsd_071536	$CoK_2O_6Se_2$	166	12.58	3.77	Γ_3^+
icsd_006152	$CoNaO_2$	166	12.58	1.31	Γ_3^+
icsd_031917	CoO_2Pd	166	12.62	0.00	Γ_3^+
icsd_031916	CoO_2Pt	166	12.58	0.00	Γ_3^+
icsd_168949	CoY	166	12.62	0.00	Γ_3^+
icsd_026676	$CrCuO_2$	166	166.101	1.77	Γ_2^+
icsd_010342	CrF_6Sr	166	166.101	0.89	Γ_2^+
icsd_670141	$CrGa_4$	166	12.62	0.00	Γ_3^+
icsd_040267	$CrKO_2$	166	166.101	2.42	Γ_2^+
icsd_025723	$CrKS_2$	166	166.101	1.59	Γ_2^+
icsd_097758	$CrLiO_2$	166	166.101	2.39	Γ_2^+
icsd_024595	$CrNaO_2$	166	166.101	1.95	Γ_2^+
icsd_015558	$CrNaS_2$	166	12.58	1.17	Γ_3^+
icsd_031679	$CrNaSe_2$	166	166.101	0.47	Γ_2^+
icsd_193884	CrO_2Pd	166	12.58	0.00	Γ_3^+
icsd_671321	CRu_2	166	166.101	0.00	Γ_2^+
icsd_028694	CsF_6Ru	166	12.58	2.10	Γ_3^+
icsd_024160	$CuFeO_2$	166	166.101	1.48	Γ_2^+
icsd_031918	$CuFeO_2$	166	166.101	1.15	Γ_2^+
icsd_028783	F_3Ti	166	166.101	1.40	Γ_2^+
icsd_028692	F_6KRu	166	12.58	1.92	Γ_3^+
icsd_061276	F_6MnRb_2	166	12.58	4.38	Γ_3^+
icsd_030114	F_6NiSr	166	166.101	0.14	Γ_2^+
icsd_028693	F_6RbRu	166	12.58	2.01	Γ_3^+
icsd_042158	F_6RhSr	166	166.101	0.22	Γ_2^+
icsd_067701	Fe_2O_4Y	166	12.62	0.00	Γ_3^+

TABLE S24. Tabulated information on **ferromagnetic** materials, including the chemical formula, space group, magnetic space group, band gap and corresponding irreducible representations of crystallographic space group.

ICSD number	Chemical formula	SG NUM	BNS	Band Gap (eV)	Irrep
icsd_000071	Fe_3Sn_2	166	166.101	0.00	Γ_2^+
icsd_670405	Fe_6Ge_4Mg	166	166.101	0.00	Γ_2^+
icsd_051207	$FeLiO_2$	166	166.101	1.62	Γ_2^+
icsd_037157	$FeNaO_2$	166	12.58	1.71	Γ_3^+
icsd_022285	$HCoO_2$	166	12.58	0.95	Γ_3^+
icsd_022108	I_2Ni	166	166.101	0.61	Γ_2^+
icsd_108894	$In_2Ni_3S_2$	166	12.58	0.00	Γ_3^+
icsd_640140	$In_2Ni_3Se_2$	166	8.34	0.00	Γ_3^+
icsd_061692	$IrKLi_6O_6$	166	166.101	0.61	Γ_2^+
icsd_071540	$K_2MnO_6Se_2$	166	166.101	3.79	Γ_2^+
icsd_165117	$K_3Mn_2O_8$	166	166.101	0.16	Γ_2^+
icsd_166489	KS_2Ti	166	12.58	0.70	Γ_3^+
icsd_641350	KS_2Zr	166	8.34	0.00	Γ_3^+
icsd_026608	$LiNiO_2$	166	12.58	0.00	Γ_3^+
icsd_024594	LiO_2V	166	12.58	1.68	Γ_3^+
icsd_189825	LiS_2Ti	166	12.58	0.00	Γ_3^+
icsd_170347	NaO_2Ru	166	12.62	0.87	Γ_3^+
icsd_043439	NaO_2Ti	166	12.58	0.45	Γ_3^+
icsd_420137	NaO_2V	166	12.58	1.79	Γ_3^+
icsd_026305	NaS_2Ti	166	12.62	0.00	Γ_3^+
icsd_076541	NaS_2V	166	12.62	1.29	Γ_3^+
icsd_077597	$NaSe_2V$	166	12.62	0.67	Γ_3^+
icsd_108892	$Ni_3Pb_2Se_2$	166	12.62	0.00	Γ_3^+
icsd_108893	$Ni_3S_2Tl_2$	166	12.58	0.00	Γ_3^+
icsd_043740	NiO	166	12.58	1.75	Γ_3^+
icsd_076959	NiO	166	12.58	1.75	Γ_3^+
icsd_025561	STi	166	12.62	0.00	Γ_3^+
icsd_030662	Ba_3NiO_4	167	15.89	1.14	Γ_3^+
icsd_043311	$BCrO_3$	167	15.85	2.13	Γ_3^+
icsd_045060	BO_3V	167	15.89	1.88	Γ_3^+
icsd_016675	F_3Pd	167	15.85	0.00	Γ_3^+
icsd_187087	$LaNiO_3$	167	15.85	0.00	Γ_3^+
icsd_150551	LiRh	174	187.213	0.00	Γ_1
icsd_080771	Ba_3MnN_3	176	11.54	0.00	$\Gamma_4^+\Gamma_6^+$
icsd_053564	Fe_3Te_3Tl	176	11.54	0.00	$\Gamma_4^+\Gamma_6^+$
icsd_100785	$LaRu_3Si_2$	176	11.54	0.00	$\Gamma_4^+\Gamma_6^+$
icsd_080772	MnN_3Sr_3	176	176.143	0.00	Γ_1^+
icsd_650662	Ru_3Si_2Y	176	176.143	0.00	Γ_1^+
icsd_079629	Se_4Ti_3	176	176.143	0.00	Γ_1^+
icsd_077371	Si_2V	180	180.171	0.00	Γ_2
icsd_096025	Si_2V	181	181.177	0.00	Γ_2
icsd_042542	CFe_3	182	182.183	0.00	Γ_2
icsd_053016	$CoNb_3S_6$	182	182.183	0.00	Γ_2
icsd_624304	$CoNb_3Se_6$	182	20.34	0.00	Γ_6
icsd_626392	$CrNb_3S_6$	182	20.34	0.00	Γ_6
icsd_626398	$CrNb_3Se_6$	182	20.34	0.00	Γ_6
icsd_626633	CrS_6Ta_3	182	20.34	0.00	Γ_6
icsd_626727	$CrSe_6Ta_3$	182	20.34	0.00	Γ_6
icsd_104913	$MnNb_3S_6$	182	182.183	0.00	Γ_2
icsd_643023	$MnNb_3Se_6$	182	20.34	0.00	Γ_6
icsd_643472	MnS_6Ta_3	182	20.34	0.00	Γ_6
icsd_645400	Nb_3Se_6V	182	20.34	0.00	Γ_6
icsd_651111	S_6Ta_3V	182	20.34	0.00	Γ_6
icsd_651970	Se_6Ta_3V	182	182.183	0.00	Γ_2
icsd_161882	$Al_{0.75}NZr_{0.25}$	186	186.207	0.00	Γ_2
icsd_168896	BTc	186	186.207	0.00	Γ_2
icsd_002064	Cl_3CsCu	186	36.174	1.35	Γ_6
icsd_024792	CrSe	186	194.270	0.00	Γ_2
icsd_060417	F_6K_2Mn	186	186.207	3.79	Γ_2
icsd_025578	F_6MnRb_2	186	36.175	4.42	Γ_6
icsd_184928	MnN	186	186.207	0.00	Γ_2
icsd_039504	$MnNa_2O_4$	186	186.207	0.51	Γ_2
icsd_649860	Pt_3Y_7	186	36.175	0.00	Γ_6
icsd_043671	CRu	187	38.191	0.00	Γ_6
icsd_104487	IrLi	187	187.213	0.00	Γ_2

TABLE S25. Tabulated information on **ferromagnetic** materials, including the chemical formula, space group, magnetic space group, band gap and corresponding irreducible representations of crystallographic space group.

ICSD number	Chemical formula	SG NUM	BNS	Band Gap (eV)	Irrep
icsd_290439	N_2Os	187	187.213	0.00	Γ_2
icsd_290430	N_2Ta	187	187.213	0.00	Γ_2
icsd_185572	NRu	187	38.189	0.00	Γ_6
icsd_182014	NTc	187	187.213	0.00	Γ_2
icsd_185568	NZr	187	187.213	0.00	Γ_2
icsd_073339	I_3LiSc	188	188.219	0.00	Γ_2
icsd_150575	Al_2CoZr_6	189	38.191	0.00	Γ_6
icsd_402701	Al_2FeZr_6	189	38.191	0.00	Γ_6
icsd_027140	$Al_8FeMg_3Si_6$	189	189.225	0.00	Γ_4
icsd_096905	$Al_9FeMg_3Si_5$	189	189.225	0.00	Γ_4
icsd_083932	As_2CoZr_6	189	189.225	0.00	Γ_4
icsd_610094	AsCoNi	189	38.189	0.00	Γ_6
icsd_043919	AsCrRh	189	38.191	0.00	Γ_6
icsd_610906	AsMnPd	189	38.191	0.00	Γ_6
icsd_044003	AsMnRh	189	189.225	0.00	Γ_4
icsd_044004	AsMnRu	189	38.191	0.00	Γ_6
icsd_020298	BFeNb	189	38.191	0.00	Γ_6
icsd_054566	Bi_2CoHf_6	189	38.189	0.00	Γ_6
icsd_240169	Bi_2CoY_6	189	189.225	0.00	Γ_4
icsd_020876	$CoGa_2Zr_6$	189	189.225	0.00	Γ_4
icsd_623801	CoHfSn	189	38.191	0.00	Γ_6
icsd_042061	CrGeNb	189	38.191	0.00	Γ_6
icsd_626517	CrPPd	189	189.225	0.00	Γ_4
icsd_061415	$Fe_2S_6Ta_9$	189	38.191	0.00	Γ_6
icsd_631770	$FeGa_2Hf_6$	189	38.191	0.00	Γ_6
icsd_631856	$FeGa_2Zr_6$	189	38.191	0.00	Γ_6
icsd_023577	FeGeHf	189	38.191	0.00	Γ_6
icsd_096249	$FeLu_6Sb_2$	189	38.191	0.00	Γ_6
icsd_096247	$FeSb_2Sc_6$	189	38.191	0.00	Γ_6
icsd_096248	$FeSb_2Y_6$	189	38.191	0.00	Γ_6
icsd_156949	$FeSb_2Zr_6$	189	38.191	0.00	Γ_6
icsd_090081	$FeSc_6Te_2$	189	38.191	0.00	Γ_6
icsd_082530	$FeTe_2Zr_6$	189	38.191	0.00	Γ_6
icsd_636559	GeHfMn	189	38.189	0.00	Γ_6
icsd_042911	GeMnNb	189	38.191	0.00	Γ_6
icsd_041156	GeMnPd	189	189.225	0.00	Γ_4
icsd_637069	GeMnRh	189	38.191	0.00	Γ_6
icsd_600156	GeMnSc	189	38.191	0.00	Γ_6
icsd_637098	GeMnTa	189	189.225	0.00	Γ_4
icsd_167625	InLaNi	189	189.225	0.00	Γ_4
icsd_411152	$Li_5N_3Ni_3$	189	38.189	0.00	Γ_6
icsd_024185	MnNbSi	189	38.191	0.00	Γ_6
icsd_600852	MnNiP	189	189.225	0.00	Γ_4
icsd_643230	MnPRh	189	189.225	0.00	Γ_4
icsd_189959	MoPRu	189	189.225	0.00	Γ_4
icsd_030416	B_2Cr	191	65.486	0.00	Γ_6^+
icsd_613892	B_2Fe	191	191.240	0.00	Γ_2^+
icsd_044439	B_2LuRu_3	191	65.486	0.00	Γ_6^+
icsd_043664	B_2Mn	191	191.240	0.00	Γ_2^+
icsd_044581	B_2Ru_3Y	191	65.486	0.00	Γ_6^+
icsd_030331	B_2V	191	65.486	0.00	Γ_6^+
icsd_036504	$BCaNi_4$	191	191.240	0.00	Γ_2^+
icsd_613036	BCo_3FeY	191	191.240	0.00	Γ_2^+
icsd_051272	BCo_4Y	191	191.240	0.00	Γ_2^+
icsd_058745	$Be_{12}Ti$	191	191.240	0.00	Γ_2^+
icsd_601122	BFe_4Lu	191	65.486	0.00	Γ_6^+
icsd_054474	$CaNi_5$	191	191.240	0.00	Γ_2^+
icsd_260251	Co_2In_9K	191	191.240	0.00	Γ_2^+
icsd_623103	Co_3Ga_2La	191	191.240	0.00	Γ_2^+
icsd_102458	Co_3Ga_2Y	191	65.486	0.00	Γ_6^+
icsd_623631	Co_6Ge_6Ti	191	191.240	0.00	Γ_2^+
icsd_055564	CoSn	191	191.240	0.00	Γ_2^+
icsd_053466	Fe_6Ge_6Hf	191	191.240	0.00	Γ_2^+
icsd_084189	Fe_6Ge_6Lu	191	191.240	0.00	Γ_2^+
icsd_041461	Fe_6Ge_6Mg	191	191.240	0.00	Γ_2^+

TABLE S26. Tabulated information on **ferromagnetic** materials, including the chemical formula, space group, magnetic space group, band gap and corresponding irreducible representations of crystallographic space group.

ICSD number	Chemical formula	SG NUM	BNS	Band Gap (eV)	Irrep
icsd_092176	Fe_6Ge_6Nb	191	191.240	0.00	Γ_2^+
icsd_092170	Fe_6Ge_6Sc	191	191.240	0.00	Γ_2^+
icsd_092172	Fe_6Ge_6Ti	191	191.240	0.00	Γ_2^+
icsd_092174	Fe_6Ge_6Zr	191	191.240	0.00	Γ_2^+
icsd_632480	Fe_6LuSn_6	191	191.240	0.00	Γ_2^+
icsd_633457	Fe_6ScSn_6	191	191.240	0.00	Γ_2^+
icsd_053459	FeGe	191	191.240	0.00	Γ_2^+
icsd_103634	FeSn	191	191.240	0.00	Γ_2^+
icsd_089433	Ge_6Mn_6Zr	191	65.486	0.00	Γ_6^+
icsd_054930	$HfMn_6Sn_6$	191	65.486	0.00	Γ_6^+
icsd_057416	$LuMn_6Sn_6$	191	65.486	0.00	Γ_6^+
icsd_015995	Mn_2O_3Ta	191	65.486	0.00	Γ_6^+
icsd_054273	Mn_6ScSn_6	191	65.486	0.00	Γ_6^+
icsd_054928	Mn_6Sn_6Zr	191	65.486	0.00	Γ_6^+
icsd_186421	N_3Ta_2Ti	191	65.486	0.00	Γ_6^+
icsd_181506	S_2Ti	191	191.240	0.00	Γ_2^+
icsd_613552	BCr_5Si_3	193	63.464	0.00	Γ_6^+
icsd_173362	Bi_5La_3Mn	193	63.464	0.00	Γ_6^+
icsd_617535	CCr_5Si_3	193	193.260	0.00	Γ_2^+
icsd_659155	$CoLa_5Pb_3$	193	63.464	0.00	Γ_6^+
icsd_604209	$CoPb_3Zr_5$	193	193.260	0.00	Γ_2^+
icsd_624928	$CoSb_3Zr_5$	193	63.464	0.00	Γ_6^+
icsd_659152	$CrLa_5Pb_3$	193	193.260	0.00	Γ_2^+
icsd_659154	$FeLa_5Pb_3$	193	193.260	0.00	Γ_2^+
icsd_604198	$FePb_3Zr_5$	193	63.464	0.00	Γ_6^+
icsd_104003	$Ga_3Ti_2Zr_3$	193	63.464	0.00	Γ_6^+
icsd_103996	Ga_3Ti_5	193	193.260	0.00	Γ_2^+
icsd_103997	Ga_4Ti_5	193	193.260	0.00	Γ_2^+
icsd_076138	Ge_3Mn_5	193	193.260	0.00	Γ_2^+
icsd_637143	Ge_3Mo_5	193	193.260	0.00	Γ_2^+
icsd_638048	Ge_3Ti_5	193	193.260	0.00	Γ_2^+
icsd_109145	I_3Nb	193	193.260	0.00	Γ_2^+
icsd_659153	La_5MnPb_3	193	63.464	0.00	Γ_6^+
icsd_168592	$La_6Mn_2S_{10}$	193	193.260	0.00	Γ_2^+
icsd_024359	Mn_5Si_3	193	63.463	0.00	Γ_6^+
icsd_644410	Mo_5Si_3	193	193.260	0.00	Γ_2^+
icsd_604200	$NiPb_3Zr_5$	193	63.463	0.00	Γ_6^+
icsd_646460	$NiSb_3Zr_5$	193	63.464	0.00	Γ_6^+
icsd_650598	$RuSb_3Zr_5$	193	193.260	0.00	Γ_2^+
icsd_044386	Si_3Ti_5	193	193.260	0.00	Γ_2^+
icsd_180888	$AgCoO_2$	194	12.62	0.00	Γ_6^+
icsd_415451	$AgNiO_2$	194	63.463	0.00	Γ_6^+
icsd_057617	Al_3CoLu_2	194	194.270	0.00	Γ_2^+
icsd_603210	$AlLa_3$	194	63.464	0.00	Γ_6^+
icsd_043888	AsCo	194	63.463	0.00	Γ_6^+
icsd_107934	AsCr	194	194.270	0.00	Γ_2^+
icsd_187133	AsFeLi	194	63.464	0.00	Γ_6^+
icsd_009497	AsMn	194	63.463	0.00	Γ_6^+
icsd_670095	$AuNiO_2$	194	194.270	0.00	Γ_2^+
icsd_670857	B_4Fe	194	63.464	0.00	Γ_6^+
icsd_035029	$BaCrO_3$	194	63.464	0.00	Γ_6^+
icsd_023874	$BaMnO_3$	194	63.463	0.02	Γ_6^+
icsd_015520	BaO_3Rh	194	194.270	0.00	Γ_2^+
icsd_010486	$BaSe_3V$	194	194.270	0.00	Γ_2^+
icsd_058805	BiMn	194	194.270	0.00	Γ_2^+
icsd_027511	Cl_3CoCs	194	63.464	2.34	Γ_6^+
icsd_024305	Cl_3CoRb	194	63.463	2.22	Γ_6^+
icsd_108289	Co_2Ge	194	63.463	0.00	Γ_6^+
icsd_053018	Co_3Nb_2Si	194	63.464	0.00	Γ_6^+
icsd_009966	Co_3Sc_2Si	194	194.270	0.00	Γ_2^+
icsd_625031	Co_3Si	194	63.464	0.00	Γ_6^+
icsd_623495	CoGeMn	194	63.464	0.00	Γ_6^+
icsd_053006	CoMnSi	194	63.464	0.00	Γ_6^+
icsd_102582	CoNiSn	194	194.270	0.00	Γ_2^+
icsd_076118	CoSb	194	63.463	0.00	Γ_6^+

TABLE S27. Tabulated information on **ferromagnetic** materials, including the chemical formula, space group, magnetic space group, band gap and corresponding irreducible representations of crystallographic space group.

ICSD number	Chemical formula	SG NUM	BNS	Band Gap (eV)	Irrep
icsd_053090	CoTe	194	194.270	0.00	Γ_2^+
icsd_053124	Cr_2GaN	194	194.270	0.00	Γ_2^+
icsd_053215	CrSe	194	194.270	0.00	Γ_2^+
icsd_053230	CrTe	194	194.270	0.00	Γ_2^+
icsd_410394	$Cs_2F_6Ni_2$	194	63.463	4.84	Γ_6^+
icsd_015092	CsF_3Ni	194	63.463	4.79	Γ_6^+
icsd_631863	$Fe_{1.5}Ga_{0.5}Zr$	194	194.270	0.00	Γ_2^+
icsd_053460	Fe_2Ge	194	191.240	0.00	Γ_2^+
icsd_409622	Fe_2ILa_2	194	63.464	0.00	Γ_6^+
icsd_103637	Fe_2Sn	194	194.270	0.00	Γ_2^+
icsd_631740	Fe_3Ga	194	63.463	0.00	Γ_6^+
icsd_023405	Fe_3Ge	194	194.270	0.00	Γ_2^+
icsd_053483	Fe_3GeZr_2	194	63.463	0.00	Γ_6^+
icsd_053558	Fe_3SiZr_2	194	63.464	0.00	Γ_6^+
icsd_024569	Fe_3Sn	194	194.270	0.00	Γ_2^+
icsd_053535	FeSb	194	194.270	0.00	Γ_2^+
icsd_181132	FeSbV	194	63.463	0.00	Γ_6^+
icsd_150620	FeSn	194	194.270	0.00	Γ_2^+
icsd_103807	GaMnPt	194	194.270	0.00	Γ_2^+
icsd_041921	GeMnNi	194	194.270	0.00	Γ_2^+
icsd_151196	$InNi_3$	194	63.463	0.00	Γ_6^+
icsd_640342	$InRu_3$	194	63.463	0.00	Γ_6^+
icsd_015908	$InSc_3$	194	194.270	0.00	Γ_2^+
icsd_108590	MnNiSi	194	63.463	0.00	Γ_6^+
icsd_073361	MnO_3Y	194	63.463	0.00	Γ_6^+
icsd_191785	MnP	194	63.464	0.00	Γ_6^+
icsd_053970	MnSb	194	194.270	0.00	Γ_2^+
icsd_670980	Nb_2Ni_3Si	194	194.270	0.00	Γ_2^+
icsd_670879	Ni_3Sn	194	194.270	0.00	Γ_2^+
icsd_189498	NiPY	194	194.270	0.00	Γ_2^+
icsd_076678	NiPZr	194	63.464	0.00	Γ_6^+
icsd_105427	NiTl	194	194.270	0.00	Γ_2^+
icsd_169821	NV	194	63.464	0.00	Γ_6^+
icsd_020009	PoTi	194	194.270	0.00	Γ_2^+
icsd_042444	PV	194	63.463	0.00	Γ_6^+
icsd_018130	Se_2Ta	194	63.463	0.00	Γ_6^+
icsd_652041	SeTi	194	194.270	0.00	Γ_2^+
icsd_052503	TeTi	194	194.270	0.00	Γ_2^+
icsd_106184	$TiZn_2$	194	63.463	0.00	Γ_6^+
icsd_020309	AsNiS	198	19.27	0.00	Γ_4
icsd_616878	BiNiSe	198	19.27	0.00	Γ_4
icsd_052963	CoGe	198	146.10	0.00	Γ_4
icsd_626558	CrPtSb	198	146.10	0.00	Γ_4
icsd_103606	FePtSb	198	19.27	0.00	Γ_4
icsd_016838	MnSi	198	146.10	0.00	Γ_4
icsd_093898	NiPS	198	19.27	0.00	Γ_4
icsd_093902	NiSbSe	198	19.27	0.00	Γ_4
icsd_652380	SiTc	198	146.10	0.00	Γ_4
icsd_043715	CoS_2	205	61.436	0.00	Γ_4^+
icsd_042539	$CoSe_2$	205	61.436	0.00	Γ_4^+
icsd_625403	$CoTe_2$	205	61.436	0.00	Γ_4^+
icsd_185888	CrO_2	205	61.436	0.00	Γ_4^+
icsd_000316	FeS_2	205	148.17	0.00	Γ_4^+
icsd_251567	IrO_2	205	1.1	0.00	Γ_4^+
icsd_290438	N_2Re	205	61.436	0.00	Γ_4^+
icsd_251565	O_2Rh	205	148.17	0.00	Γ_4^+
icsd_181055	$Cd_{0.25}Cr_{0.75}Te$	215	160.67	0.00	Γ_5
icsd_181053	$Cd_{0.75}Cr_{0.25}Te$	215	160.67	0.00	Γ_5
icsd_181035	$Cr_{0.25}Ga_{0.75}P$	215	111.255	0.00	Γ_5
icsd_186188	$Cr_{0.25}SeZn_{0.75}$	215	111.255	0.00	Γ_5
icsd_186187	$Cr_{0.25}SZn_{0.75}$	215	111.255	0.00	Γ_5
icsd_186189	$Cr_{0.25}TeZn_{0.75}$	215	111.255	0.00	Γ_5
icsd_181036	$Cr_{0.75}Ga_{0.25}P$	215	160.67	0.00	Γ_5
icsd_629351	Cu_3Te_4V	215	111.255	0.19	Γ_5
icsd_189696	$AlTi_2$	216	119.319	0.00	Γ_5

TABLE S28. Tabulated information on **ferromagnetic** materials, including the chemical formula, space group, magnetic space group, band gap and corresponding irreducible representations of crystallographic space group.

ICSD number	Chemical formula	SG NUM	BNS	Band Gap (eV)	Irrep
icsd_185882	$AlTi_2Zn$	216	119.319	0.00	Γ_5
icsd_192816	AsLiMn	216	44.231	0.00	Γ_5
icsd_184925	AsMn	216	44.231	0.00	Γ_5
icsd_161716	AsMnNi	216	119.319	0.10	Γ_5
icsd_052673	AuMnSb	216	119.319	0.00	Γ_5
icsd_054465	AuMnSn	216	44.231	0.00	Γ_5
icsd_671366	BiCoPt	216	44.231	0.00	Γ_5
icsd_671365	BiFePt	216	44.231	0.00	Γ_5
icsd_671364	BiMnPt	216	160.67	0.00	Γ_5
icsd_671367	BiNiPt	216	160.67	0.00	Γ_5
icsd_168901	BTc	216	160.67	0.00	Γ_5
icsd_190995	$CMnSc_2$	216	44.231	0.00	Γ_5
icsd_183166	CMo	216	216.75	0.00	Γ_5
icsd_623808	Co_2HfSn	216	139.537	0.00	Γ_5
icsd_625319	Co_2SnZr	216	139.537	0.00	Γ_5
icsd_670706	CoFeSiZr	216	160.67	0.00	Γ_5
icsd_108294	CoHfSb	216	44.231	0.00	Γ_5
icsd_079936	CoN	216	119.319	0.00	Γ_5
icsd_107129	CoNbSb	216	119.319	0.00	Γ_5
icsd_102552	CoNbSn	216	44.231	0.00	Γ_5
icsd_029082	CoO	216	119.319	0.80	Γ_5
icsd_108317	CoSbZr	216	44.231	0.00	Γ_5
icsd_106496	CoSnTi	216	44.231	0.00	Γ_5
icsd_181079	CrN	216	160.67	0.00	Γ_5
icsd_671343	CrSe	216	160.67	0.00	Γ_5
icsd_169766	CrTe	216	44.231	0.00	Γ_5
icsd_169407	CSc	216	44.231	0.00	Γ_5
icsd_183168	CTc	216	119.319	0.00	Γ_5
icsd_042978	CuMnSb	216	44.231	0.00	Γ_5
icsd_183160	CY	216	160.67	0.00	Γ_5
icsd_041258	FeN	216	119.319	0.00	Γ_5
icsd_083928	FeNbSb	216	119.319	0.00	Γ_5
icsd_090397	FeSbZn	216	44.231	0.00	Γ_5
icsd_108482	GaMnPt	216	119.319	0.00	Γ_5
icsd_108492	GaRhTi	216	160.67	0.00	Γ_5
icsd_189699	$GaTi_2$	216	119.319	0.00	Γ_5
icsd_161715	GeMnNi	216	160.67	0.00	Γ_5
icsd_190999	$GeMnSc_2$	216	44.231	0.00	Γ_5
icsd_169409	GeSc	216	160.67	0.00	Γ_5
icsd_189708	$GeTi_2$	216	160.67	0.00	Γ_5
icsd_189702	$InTi_2$	216	44.231	0.00	Γ_5
icsd_104498	IrMnSn	216	160.67	0.00	Γ_5
icsd_236787	MnN	216	160.67	0.00	Γ_5
icsd_054255	MnNiSb	216	44.231	0.00	Γ_5
icsd_161713	MnNiSi	216	44.231	0.00	Γ_5
icsd_191788	MnP	216	119.319	0.00	Γ_5
icsd_643329	$MnPd_2Sn$	216	139.537	0.00	Γ_5
icsd_076099	MnPdSb	216	44.231	0.00	Γ_5
icsd_040908	MnPdTe	216	119.319	0.00	Γ_5
icsd_057421	MnPtSb	216	160.67	0.00	Γ_5
icsd_104955	MnPtSn	216	160.67	0.00	Γ_5
icsd_076205	MnS	216	44.231	1.13	Γ_5
icsd_191175	MnSb	216	119.319	0.00	Γ_5
icsd_190997	$MnSc_2Si$	216	160.67	0.00	Γ_5
icsd_191001	$MnSc_2Sn$	216	44.231	0.00	Γ_5
icsd_024252	MnSe	216	160.67	0.82	Γ_5
icsd_191171	MnSn	216	119.319	0.00	Γ_5
icsd_181324	MnTe	216	44.231	0.52	Γ_5
icsd_159438	MoN	216	119.319	0.00	Γ_5
icsd_186876	MoP	216	160.67	0.00	Γ_5
icsd_107122	NbRhSb	216	44.231	0.00	Γ_5
icsd_105220	NbRhSn	216	119.319	0.00	Γ_5
icsd_076699	NiSbTi	216	119.319	0.00	Γ_5
icsd_054259	NiSnTi	216	8.32	0.00	Γ_5
icsd_161755	NNi	216	119.319	0.00	Γ_5

TABLE S29. Tabulated information on **ferromagnetic** materials, including the chemical formula, space group, magnetic space group, band gap and corresponding irreducible representations of crystallographic space group.

ICSD number	Chemical formula	SG NUM	BNS	Band Gap (eV)	Irrep
icsd_167870	NTc	216	44.231	0.00	Γ_5
icsd_236783	NV	216	160.67	0.10	Γ_5
icsd_167877	NW	216	119.319	0.00	Γ_5
icsd_169408	ScSi	216	44.231	0.00	Γ_5
icsd_169410	ScSn	216	119.319	0.00	Γ_5
icsd_671386	SeV	216	44.231	0.00	Γ_5
icsd_189705	$SiTi_2$	216	44.231	0.00	Γ_5
icsd_189711	$SnTi_2$	216	44.231	0.00	Γ_5
icsd_671387	TeV	216	160.67	0.00	Γ_5
icsd_167814	Al_3Ti	221	8.34	0.00	Γ_4^+
icsd_167812	Al_3V	221	123.345	0.00	Γ_4^+
icsd_187962	$AlCo_3$	221	65.486	0.00	Γ_4^+
icsd_057932	$AlLa_3$	221	123.345	0.00	Γ_4^+
icsd_608581	AlMo	221	123.345	0.00	Γ_4^+
icsd_058038	$AlNi_3$	221	123.345	0.00	Γ_4^+
icsd_029096	$BaFeO_3$	221	123.345	0.00	Γ_4^+
icsd_043799	$BaMoO_3$	221	123.345	0.00	Γ_4^+
icsd_237730	BaO_3Os	221	65.486	0.00	Γ_4^+
icsd_671086	BaO_3Tc	221	123.345	0.00	Γ_4^+
icsd_191203	BaO_3V	221	123.345	0.00	Γ_4^+
icsd_044430	$BLaRh_3$	221	8.34	0.00	Γ_4^+
icsd_168900	BTc	221	65.486	0.00	Γ_4^+
icsd_168902	$CaMnO_3$	221	123.345	0.00	Γ_4^+
icsd_671082	CaO_3Tc	221	123.345	0.00	Γ_4^+
icsd_108129	CCo_3Sn	221	47.252	0.00	Γ_4^+
icsd_076797	CCo_3Zn	221	47.252	0.00	Γ_4^+
icsd_422858	$CdCo_3N$	221	10.46	0.00	Γ_4^+
icsd_033667	CdO_3Ti	221	123.345	0.00	Γ_4^+
icsd_023167	Cl_3MnTl	221	65.486	2.69	Γ_4^+
icsd_077154	CMn_3Zn	221	47.252	0.00	Γ_4^+
icsd_015246	CoF_3K	221	166.101	3.06	Γ_4^+
icsd_102423	CoGa	221	65.486	0.00	Γ_4^+
icsd_028921	$CoLaO_3$	221	123.345	0.00	Γ_4^+
icsd_236831	CoN	221	123.345	0.00	Γ_4^+
icsd_077142	CoO_3Sr	221	65.486	0.00	Γ_4^+
icsd_028930	$CrLaO_3$	221	123.345	1.25	Γ_4^+
icsd_236825	CrN	221	123.345	0.00	Γ_4^+
icsd_160196	CrO_3Pb	221	166.101	0.00	Γ_4^+
icsd_108903	CrO_3Sr	221	123.345	0.00	Γ_4^+
icsd_049583	CsF_3Fe	221	166.101	3.04	Γ_4^+
icsd_042930	CTi_3Tl	221	65.486	0.00	Γ_4^+
icsd_015424	F_3FeK	221	166.101	2.86	Γ_4^+
icsd_049586	F_3FeRb	221	166.101	2.90	Γ_4^+
icsd_015423	F_3KMn	221	65.486	2.60	Γ_4^+
icsd_015426	F_3KNi	221	166.101	3.70	Γ_4^+
icsd_073167	F_3KPd	221	65.486	0.35	Γ_4^+
icsd_028145	F_3KV	221	123.345	2.05	Γ_4^+
icsd_043722	F_3MnRb	221	123.345	2.93	Γ_4^+
icsd_030612	F_3Mo	221	65.486	1.12	Γ_4^+
icsd_060611	F_3NaV	221	166.101	0.27	Γ_4^+
icsd_025596	F_3Nb	221	123.345	0.00	Γ_4^+
icsd_671397	F_3NiRb	221	65.486	3.68	Γ_4^+
icsd_073166	F_3PdRb	221	65.486	0.43	Γ_4^+
icsd_028146	F_3RbV	221	123.345	2.47	Γ_4^+
icsd_030613	F_3Ta	221	166.101	0.00	Γ_4^+
icsd_077369	$Fe_{11}Si_5$	221	123.345	0.00	Γ_4^+
icsd_103451	Fe_3Ga	221	65.486	0.00	Γ_4^+
icsd_053461	Fe_3Ge	221	166.101	0.00	Γ_4^+
icsd_103638	Fe_3Sn	221	65.486	0.00	Γ_4^+
icsd_029118	$FeLaO_3$	221	166.101	0.49	Γ_4^+
icsd_236829	FeN	221	166.101	0.00	Γ_4^+
icsd_091062	FeO_3Sr	221	123.345	0.00	Γ_4^+
icsd_103765	$GaLa_3$	221	123.345	0.00	Γ_4^+
icsd_103856	$GaNi_3$	221	65.486	0.00	Γ_4^+
icsd_103950	GaRu	221	5.15	0.00	Γ_4^+

TABLE S30. Tabulated information on **ferromagnetic** materials, including the chemical formula, space group, magnetic space group, band gap and corresponding irreducible representations of crystallographic space group.

ICSD number	Chemical formula	SG NUM	BNS	Band Gap (eV)	Irrep
icsd_168838	$H_2Mg_{0.75}Ti_{0.25}$	221	65.486	0.00	Γ_4^+
icsd_183420	HfN	221	123.345	0.00	Γ_4^+
icsd_051950	$InLa_3$	221	166.101	0.00	Γ_4^+
icsd_059438	$InNi_3$	221	166.101	0.00	Γ_4^+
icsd_042929	$InNTi_3$	221	65.486	0.00	Γ_4^+
icsd_059523	$InSc_3$	221	123.345	0.00	Γ_4^+
icsd_104722	La_3Sn	221	123.345	0.00	Γ_4^+
icsd_104732	La_3Tl	221	166.101	0.00	Γ_4^+
icsd_029119	$LaMnO_3$	221	65.486	0.00	Γ_4^+
icsd_028908	LaO_3Ti	221	123.345	0.00	Γ_4^+
icsd_028925	LaO_3V	221	166.101	0.00	Γ_4^+
icsd_187256	MgNi	221	166.101	0.00	Γ_4^+
icsd_236827	MnN	221	166.101	0.00	Γ_4^+
icsd_188415	MnO_3Sr	221	123.345	0.00	Γ_4^+
icsd_191174	MnSb	221	123.345	0.00	Γ_4^+
icsd_191170	MnSn	221	123.345	0.00	Γ_4^+
icsd_159440	MoN	221	123.345	0.00	Γ_4^+
icsd_071994	MoO_3Sr	221	166.101	0.00	Γ_4^+
icsd_236833	NNi	221	166.101	0.00	Γ_4^+
icsd_187710	NTc	221	65.486	0.00	Γ_4^+
icsd_183416	NTi	221	65.486	0.00	Γ_4^+
icsd_042931	NTi_3Tl	221	123.345	0.00	Γ_4^+
icsd_181144	NZr	221	166.101	0.00	Γ_4^+
icsd_187637	O_3PbV	221	123.345	0.00	Γ_4^+
icsd_187483	O_3RhSr	221	123.345	0.00	Γ_4^+
icsd_069360	O_3RuSr	221	166.101	0.00	Γ_4^+
icsd_109076	O_3SrTc	221	123.345	0.00	Γ_4^+
icsd_088982	O_3SrV	221	123.345	0.00	Γ_4^+
icsd_611501	$AsTi_3$	223	167.107	0.00	Γ_4^+
icsd_638098	Ge_3V	223	131.441	0.00	Γ_4^+
icsd_043356	$SbTi_3$	223	167.107	0.00	Γ_4^+
icsd_106108	$SnZr_3$	223	1.1	0.00	Γ_4^+
icsd_077714	OZr_2	224	134.477	0.00	Γ_4^+
icsd_057504	$AlAu_2Mn$	225	166.101	0.00	Γ_4^+
icsd_057507	$AlAu_2Ti$	225	8.32	0.00	Γ_4^+
icsd_057607	$AlCo_2Fe$	225	139.537	0.00	Γ_4^+
icsd_057611	$AlCo_2Hf$	225	139.537	0.00	Γ_4^+
icsd_057618	$AlCo_2Mn$	225	166.101	0.00	Γ_4^+
icsd_057620	$AlCo_2Nb$	225	139.537	0.00	Γ_4^+
icsd_057634	$AlCo_2Ta$	225	139.537	0.00	Γ_4^+
icsd_057653	$AlCrCu_2$	225	166.101	0.00	Γ_4^+
icsd_057662	$AlCrNi_2$	225	139.537	0.00	Γ_4^+
icsd_057695	$AlCu_2Mn$	225	166.101	0.00	Γ_4^+
icsd_057793	$AlFe_3$	225	166.101	0.00	Γ_4^+
icsd_057976	$AlMnNi_2$	225	166.101	0.00	Γ_4^+
icsd_057981	$AlMnPd_2$	225	166.101	0.00	Γ_4^+
icsd_057985	$AlMnPt_2$	225	166.101	0.00	Γ_4^+
icsd_057986	$AlMnRh_2$	225	166.101	0.00	Γ_4^+
icsd_058071	$AlNi_2V$	225	166.101	0.00	Γ_4^+
icsd_608800	$AlNi_3$	225	166.101	0.00	Γ_4^+
icsd_185119	$AlTiZr_2$	225	139.537	0.00	Γ_4^+
icsd_107955	$AsMnPd_2$	225	166.101	0.00	Γ_4^+
icsd_058510	Au_2InTi	225	166.101	0.00	Γ_4^+
icsd_168899	BTc	225	139.537	0.00	Γ_4^+
icsd_057008	CCr	225	166.101	0.00	Γ_4^+
icsd_185983	CIr	225	139.537	0.00	Γ_4^+
icsd_190994	$CMnSc_2$	225	71.536	0.00	Γ_4^+
icsd_180457	CNi	225	8.34	0.00	Γ_4^+
icsd_102386	Co_2FeGa	225	139.537	0.00	Γ_4^+
icsd_185936	Co_2FeGe	225	71.536	0.00	Γ_4^+
icsd_102392	Co_2FeIn	225	139.537	0.00	Γ_4^+
icsd_052958	Co_2FeSi	225	139.537	0.00	Γ_4^+
icsd_102438	Co_2GaMn	225	166.101	0.00	Γ_4^+
icsd_102441	Co_2GaNb	225	139.537	0.00	Γ_4^+
icsd_102451	Co_2GaTa	225	139.537	0.00	Γ_4^+

TABLE S31. Tabulated information on **ferromagnetic** materials, including the chemical formula, space group, magnetic space group, band gap and corresponding irreducible representations of crystallographic space group.

ICSD number	Chemical formula	SG NUM	BNS	Band Gap (eV)	Irrep
icsd_052971	Co_2GeMn	225	166.101	0.00	Γ_4^+
icsd_102483	Co_2HfSn	225	139.537	0.00	Γ_4^+
icsd_053002	Co_2MnSb	225	139.537	0.00	Γ_4^+
icsd_053007	Co_2MnSi	225	139.537	0.00	Γ_4^+
icsd_102531	Co_2MnSn	225	166.101	0.00	Γ_4^+
icsd_102554	Co_2NbSn	225	71.536	0.00	Γ_4^+
icsd_053086	Co_2SiV	225	166.101	0.00	Γ_4^+
icsd_102687	Co_2SnZr	225	139.537	0.00	Γ_4^+
icsd_623481	$Co_{8.8}Ge_4Mn_{3.2}$	225	139.537	0.00	Γ_4^+
icsd_151207	$CoCu_2Sn$	225	71.536	0.00	Γ_4^+
icsd_102385	$CoFe_2Ga$	225	166.101	0.00	Γ_4^+
icsd_052954	$CoFe_2Ge$	225	166.101	0.00	Γ_4^+
icsd_184377	CoN	225	71.536	0.00	Γ_4^+
icsd_009865	CoO	225	166.101	1.68	Γ_4^+
icsd_181773	CRh	225	139.537	0.00	Γ_4^+
icsd_037412	CrN	225	139.537	0.00	Γ_4^+
icsd_109296	CrO	225	139.537	0.00	Γ_4^+
icsd_186838	CrO_2	225	71.536	0.41	Γ_4^+
icsd_169767	CrTe	225	71.536	0.00	Γ_4^+
icsd_183167	CTc	225	139.537	0.00	Γ_4^+
icsd_151206	Cu_2FeSn	225	166.101	0.00	Γ_4^+
icsd_102996	Cu_2InMn	225	166.101	0.00	Γ_4^+
icsd_054597	Cu_2InTi	225	166.101	0.00	Γ_4^+
icsd_053312	Cu_2MnSb	225	166.101	0.00	Γ_4^+
icsd_103057	Cu_2MnSn	225	166.101	0.00	Γ_4^+
icsd_061323	CuO	225	71.536	0.00	Γ_4^+
icsd_065410	F_2Ti	225	71.536	2.03	Γ_4^+
icsd_186065	Fe_2GeMn	225	166.101	0.00	Γ_4^+
icsd_186061	Fe_2MnSi	225	166.101	0.00	Γ_4^+
icsd_108436	Fe_3Ga	225	139.537	0.00	Γ_4^+
icsd_053462	Fe_3Ge	225	71.536	0.00	Γ_4^+
icsd_053545	Fe_3Si	225	139.537	0.00	Γ_4^+
icsd_187492	$FeGaNi_2$	225	71.536	0.00	Γ_4^+
icsd_184375	FeN	225	166.101	0.00	Γ_4^+
icsd_027856	FeO	225	71.536	1.06	Γ_4^+
icsd_053525	$FeRu_2Si$	225	166.101	0.00	Γ_4^+
icsd_103615	$FeRu_2Sn$	225	166.101	0.00	Γ_4^+
icsd_670177	$FeSi_2$	225	139.537	0.00	Γ_4^+
icsd_155336	$Ga_4Mn_4Ni_8$	225	166.101	0.00	Γ_4^+
icsd_103803	$GaMnNi_2$	225	166.101	0.00	Γ_4^+
icsd_191168	$GaMnPt_2$	225	166.101	0.00	Γ_4^+
icsd_103892	$GaNi_2V$	225	166.101	0.00	Γ_4^+
icsd_053687	$GeMnNi_2$	225	166.101	0.00	Γ_4^+
icsd_053705	$GeMnPd_2$	225	139.537	0.00	Γ_4^+
icsd_053706	$GeMnRh_2$	225	166.101	0.00	Γ_4^+
icsd_190998	$GeMnSc_2$	225	139.537	0.00	Γ_4^+
icsd_056182	H_2Ti	225	166.101	0.00	Γ_4^+
icsd_056191	H_2V	225	139.537	0.00	Γ_4^+
icsd_051984	$InMnNi_2$	225	166.101	0.00	Γ_4^+
icsd_051988	$InMnPd_2$	225	166.101	0.00	Γ_4^+
icsd_054596	$InNi_2Ti$	225	139.537	0.00	Γ_4^+
icsd_104980	Mn_2SnW	225	166.101	0.00	Γ_4^+
icsd_236807	MnN	225	139.537	0.00	Γ_4^+
icsd_076080	$MnNi_2Sb$	225	166.101	0.00	Γ_4^+
icsd_104926	$MnNi_2Sn$	225	166.101	0.00	Γ_4^+
icsd_009864	MnO	225	139.537	0.25	Γ_4^+
icsd_104936	$MnPbRh_2$	225	166.101	0.00	Γ_4^+
icsd_076100	$MnPd_2Sb$	225	166.101	0.00	Γ_4^+
icsd_104945	$MnPd_2Sn$	225	139.537	0.00	Γ_4^+
icsd_104964	$MnRh_2Sn$	225	166.101	0.00	Γ_4^+
icsd_018007	MnS	225	139.537	0.71	Γ_4^+
icsd_191173	MnSb	225	166.101	0.00	Γ_4^+
icsd_190996	$MnSc_2Si$	225	139.537	0.00	Γ_4^+
icsd_191000	$MnSc_2Sn$	225	71.536	0.00	Γ_4^+
icsd_024251	MnSe	225	139.537	0.33	Γ_4^+

TABLE S32. Tabulated information on **ferromagnetic** materials, including the chemical formula, space group, magnetic space group, band gap and corresponding irreducible representations of crystallographic space group.

ICSD number	Chemical formula	SG NUM	BNS	Band Gap (eV)	Irrep
icsd_191169	MnSn	225	71.536	0.00	Γ_4^+
icsd_076240	MnTe	225	166.101	0.00	Γ_4^+
icsd_186875	MoP	225	166.101	0.00	Γ_4^+
icsd_076700	Ni_2SbTi	225	225.117	0.00	Γ_4^+
icsd_105376	Ni_2SnV	225	139.537	0.00	Γ_4^+
icsd_009866	NiO	225	71.536	1.75	Γ_4^+
icsd_105327	$NiRh_2Sn$	225	139.537	0.00	Γ_4^+
icsd_169573	NiS_2	225	139.537	0.00	Γ_4^+
icsd_236813	NNi	225	71.536	0.00	Γ_4^+
icsd_167863	NOs	225	139.537	0.00	Γ_4^+
icsd_167855	NRu	225	166.101	0.00	Γ_4^+
icsd_167854	NTc	225	166.101	0.00	Γ_4^+
icsd_022321	NV	225	71.536	0.00	Γ_4^+
icsd_077650	OPd	225	139.537	0.00	Γ_4^+
icsd_040125	OTi	225	71.536	0.00	Γ_4^+
icsd_028681	OV	225	139.537	0.00	Γ_4^+
icsd_105933	Rh_2SnV	225	166.101	0.00	Γ_4^+
icsd_424636	Ga_4Mn	229	166.101	0.00	Γ_4^+
icsd_027836	O_4Pt_3	229	166.101	0.00	Γ_4^+

C. Collinear Ferrimagnetic Materials

The relevant information for ferrimagnetic materials is summarized in Table S33-S36, including their chemical formula, space group, magnetic space group, band gap and corresponding irreducible representations of crystallographic space group.

TABLE S33. Tabulated information on **collinear ferrimagnetic** materials, including the chemical formula, space group, magnetic space group, band gap and corresponding irreducible representations of crystallographic space group.

ICSD number	Chemical formula	SG NUM	BNS	Band Gap (eV)	Irrep
icsd_010509	$Al_{11}Mn_4$	2	2.4	0.00	Γ_1^+
icsd_063057	$As_2Cu_3O_8$	2	2.4	2.05	Γ_1^+
icsd_167202	$CoFLiO_4S$	2	2.4	3.41	Γ_1^+
icsd_050507	CrF_6Mo	2	2.4	0.62	Γ_1^+
icsd_193472	$Cu_3Nb_2O_8$	2	2.4	0.20	Γ_1^+
icsd_001143	$Cu_3O_8P_2$	2	2.4	2.07	Γ_1^+
icsd_050506	CuF_6Mo	2	2.4	0.70	Γ_1^+
icsd_079695	$H_2As_2CuFe_2O_{10}$	2	1.1	2.55	Γ_1^-
icsd_192247	CoY_3	4	4.9	0.00	Γ_2
icsd_240499	BrOTi	11	11.54	0.00	Γ_2^+
icsd_051677	$H_3ClCu_2O_3$	11	11.54	1.70	Γ_2^+
icsd_624485	Co_2NiSe_4	12	12.62	0.00	Γ_2^+
icsd_622499	$CoCr_2S_4$	12	12.62	0.00	Γ_2^+
icsd_601038	$CoCr_2Se_4$	12	12.62	0.00	Γ_2^+
icsd_622979	$CoFe_2Se_4$	12	12.62	0.00	Γ_2^+
icsd_026173	$CoMo_2S_4$	12	12.58	0.00	Γ_1^+
icsd_624874	CoS_4Ti_2	12	12.62	0.00	Γ_2^+
icsd_624884	CoS_4V_2	12	12.58	0.00	Γ_1^+
icsd_625002	$CoSe_4Ti_2$	12	12.62	0.00	Γ_2^+
icsd_625012	$CoSe_4V_2$	12	12.58	0.00	Γ_1^+
icsd_625931	Cr_2FeS_4	12	12.62	0.27	Γ_2^+
icsd_043042	Cr_2FeSe_4	12	12.62	0.00	Γ_2^+
icsd_016884	Cr_2NiS_4	12	12.62	0.06	Γ_2^+
icsd_626655	CrS_4V_2	12	12.58	0.00	Γ_1^+
icsd_633332	$Fe_{0.5}S_2Ti$	12	12.62	0.00	Γ_2^+
icsd_015043	Fe_3Se_4	12	12.62	0.00	Γ_2^+
icsd_632972	$FeNi_2Se_4$	12	12.62	0.00	Γ_2^+
icsd_603354	$FeRh_2Se_4$	12	12.58	0.00	Γ_1^+
icsd_042563	FeS_4Ti_2	12	12.62	0.00	Γ_2^+
icsd_035634	FeS_4V_2	12	12.62	0.06	Γ_2^+
icsd_633504	$FeSe_4Ti_2$	12	12.62	0.61	Γ_2^+
icsd_193869	$Ni_{0.5}Se_2Ti$	12	12.62	0.00	Γ_2^+
icsd_042558	Ni_3Se_4	12	12.62	0.00	Γ_2^+
icsd_646388	NiS_4Ti_2	12	12.62	0.00	Γ_2^+
icsd_035140	NiS_4V_2	12	12.62	0.00	Γ_2^+
icsd_646544	$NiSe_4Ti_2$	12	12.62	0.00	Γ_2^+
icsd_023970	$NiSe_4V_2$	12	12.62	0.00	Γ_2^+
icsd_024566	S_4V_3	12	12.62	0.00	Γ_2^+
icsd_601347	Se_4Ti_3	12	12.58	0.00	Γ_1^+
icsd_043412	Te_4Ti_3	12	12.58	0.00	Γ_1^+
icsd_041858	AsCoS	14	14.75	0.00	Γ_1^+
icsd_239671	Ca_2CrO_6Os	14	14.79	0.00	Γ_2^+
icsd_089955	Ca_2FeMoO_6	14	14.75	0.67	Γ_1^+
icsd_238148	Ca_2FeO_6Os	14	14.75	0.72	Γ_1^+
icsd_181147	$FeMn_2O_6Sb$	14	14.79	1.53	Γ_2^+
icsd_096120	La_2NiO_6Ru	14	14.79	0.76	Γ_2^+
icsd_252567	Mn_3O_6Re	14	14.79	0.00	Γ_2^+
icsd_602022	HFeTi	17	51.296	0.00	Γ_3
icsd_632217	H_2FeTi	26	26.69	0.00	Γ_3
icsd_627741	$Cu_2GeMnSe_4$	31	31.127	1.01	Γ_2
icsd_020082	AlB_4Cr_3	47	47.252	0.00	Γ_4^+
icsd_171434	$BaCo_2O_5Y$	51	51.296	0.48	Γ_4^+
icsd_033996	$CoCu_2O_3$	59	59.410	0.68	Γ_4^+
icsd_610884	AsMnNi	62	62.446	0.00	Γ_2^+
icsd_670822	CCo_2Fe	62	62.446	0.00	Γ_2^+
icsd_670825	$CCrFe_2$	62	62.441	0.00	Γ_1^+
icsd_167127	CFe_2Ni	62	62.446	0.00	Γ_2^+
icsd_025726	Co_2P	62	62.447	0.00	Γ_3^+
icsd_016483	CoMnP	62	62.448	0.00	Γ_4^+
icsd_005432	CoMnSi	62	62.446	0.00	Γ_2^+
icsd_002421	CoMoP	62	62.446	0.00	Γ_2^+
icsd_624646	CoPTi	62	62.446	0.00	Γ_2^+
icsd_041918	GeMnNi	62	62.447	0.00	Γ_3^+
icsd_076084	MnNiSi	62	62.448	0.00	Γ_4^+
icsd_187466	O_3Ti_2	62	62.446	0.30	Γ_2^+

TABLE S34. Tabulated information on **collinear ferrimagnetic** materials, including the chemical formula, space group, magnetic space group, band gap and corresponding irreducible representations of crystallographic space group.

ICSD number	Chemical formula	SG NUM	BNS	Band Gap (eV)	Irrep
icsd_044188	B_3CoV	63	63.463	0.00	Γ_3^+
icsd_042629	CCr_3Ge	63	63.464	0.00	Γ_4^+
icsd_189439	Fe_2O_3	63	63.464	0.59	Γ_4^+
icsd_065881	$BaCu_3O_4$	65	65.485	1.22	Γ_2^+
icsd_050089	$Cu_6O_{10}Sr_4$	65	65.485	0.00	Γ_2^+
icsd_044293	B_4Fe_2Mo	71	71.536	0.00	Γ_2^+
icsd_614748	B_4Mn_2Mo	71	71.536	0.00	Γ_2^+
icsd_670346	$CaMnO_3$	71	71.536	0.13	Γ_3^+
icsd_416904	$Cu_3O_5Sr_2$	71	71.536	0.37	Γ_3^+
icsd_150701	$FeMoO_6Sr_2$	87	12.62	0.00	$\Gamma_3^+\Gamma_4^+$
icsd_052332	Sb_4V_5	87	12.62	0.00	$\Gamma_3^+\Gamma_4^+$
icsd_042881	Te_4V_5	87	12.62	0.00	$\Gamma_3^+\Gamma_4^+$
icsd_067978	$BaCuFeO_5Y$	99	25.59	0.00	Γ_5
icsd_167196	$FeSe_{0.875}$	99	25.59	0.00	Γ_5
icsd_023779	CrNNb	100	99.167	0.00	Γ_4
icsd_202705	F_6Fe_2Li	102	34.158	1.49	Γ_5
icsd_067711	$Ba_2Fe_3O_8Y$	123	47.252	0.00	Γ_5^+
icsd_015521	$ClFe_3O_8Pb_4$	123	65.486	0.10	Γ_5^+
icsd_053505	FeNNi	123	65.486	0.00	Γ_5^+
icsd_613327	$B_2Co_5Ta_3$	127	65.486	0.00	Γ_5^+
icsd_614755	B_2MnMo_2	127	55.358	0.00	Γ_5^+
icsd_088317	B_2V_3	127	65.486	0.00	Γ_5^+
icsd_059553	In_4Ti_3	127	55.358	0.00	Γ_5^+
icsd_644412	Mo_3Si_2	127	65.486	0.00	Γ_5^+
icsd_016844	$AsFe_2$	129	59.410	0.00	Γ_5^+
icsd_093237	AsFeMn	129	129.417	0.00	Γ_3^+
icsd_165984	$AsFeO_3Sr_2V$	129	59.410	0.00	Γ_5^+
icsd_042329	$AsMn_2$	129	129.417	0.00	Γ_3^+
icsd_042325	Mn_2Sb	129	129.417	0.00	Γ_3^+
icsd_200014	MoO_6Rh_2	136	136.501	0.00	Γ_3^+
icsd_032011	$As_2Ba_2Mn_3O_2$	139	139.537	0.00	Γ_3^+
icsd_032010	$As_2Mn_3O_2Sr_2$	139	139.537	0.00	Γ_3^+
icsd_246541	Ba_2FeMoO_6	139	139.537	0.00	Γ_3^+
icsd_032013	$Ba_2Mn_3O_2Sb_2$	139	139.537	0.00	Γ_3^+
icsd_032014	$Bi_2Mn_3O_2Sr_2$	139	139.537	0.00	Γ_3^+
icsd_617225	$BiTi_2$	139	71.536	0.00	Γ_5^+
icsd_094079	$FeMoO_6Sr_2$	139	139.537	0.00	Γ_3^+
icsd_084202	Mn_3N_2	139	69.524	0.00	Γ_5^+
icsd_032012	$Mn_3O_2Sb_2Sr_2$	139	139.537	0.00	Γ_3^+
icsd_188743	MoO_6OsPb_2	139	139.537	0.00	Γ_3^+
icsd_188742	MoO_6OsSn_2	139	139.537	0.00	Γ_3^+
icsd_246426	Bi_2CrFeO_6	146	146.10	1.41	Γ_1
icsd_031853	$MnNiO_3$	148	2.4	0.90	$\Gamma_2^+\Gamma_3^+$
icsd_626435	CrNiP	150	38.189	0.00	Γ_3
icsd_029132	F_3Fe	150	5.13	0.00	Γ_3
icsd_029134	F_3Rh	150	5.15	0.00	Γ_3
icsd_155025	$Fe_2In_2Se_5$	164	2.4	0.00	Γ_3^+
icsd_062661	$Mn_3Nb_6O_{11}$	164	12.58	0.25	Γ_3^+
icsd_076020	O_2PTi_3	164	164.89	0.00	Γ_2^+
icsd_670856	B_4Fe	187	187.213	0.00	Γ_2
icsd_610130	$AsCr_2$	189	189.225	0.00	Γ_4
icsd_043913	AsCrNi	189	189.225	0.00	Γ_4
icsd_610275	AsCrTi	189	189.225	0.00	Γ_4
icsd_610883	AsMnNi	189	38.191	0.00	Γ_6
icsd_610927	AsMnTi	189	189.225	0.00	Γ_4
icsd_042943	CoGeTi	189	38.191	0.00	Γ_6
icsd_600596	CrNiP	189	38.191	0.00	Γ_6
icsd_043394	Mn_2P	189	38.191	0.00	Γ_6
icsd_643671	MnSiTi	189	189.225	0.00	Γ_4
icsd_614407	BGe_3V_5	193	63.464	0.00	Γ_6^+
icsd_609885	CAs_3V_5	193	63.464	0.00	Γ_6^+
icsd_042585	Fe_5Si_3	193	193.260	0.00	Γ_2^+
icsd_643689	$Mn_3Si_3V_2$	193	193.260	0.00	Γ_2^+
icsd_182095	B_4Mo	194	63.463	0.00	Γ_6^+
icsd_624067	Co_2Mg	194	63.464	0.00	Γ_6^+

TABLE S35. Tabulated information on **collinear ferrimagnetic** materials, including the chemical formula, space group, magnetic space group, band gap and corresponding irreducible representations of crystallographic space group.

ICSD number	Chemical formula	SG NUM	BNS	Band Gap (eV)	Irrep
icsd_102673	Co_2Sn	194	194.270	0.00	Γ_2^+
icsd_189226	Co_3SiTi_2	194	11.54	0.00	Γ_6^+
icsd_163332	Mn_2Sb	194	187.213	0.00	Γ_2^+
icsd_670785	AlCrHfV	216	160.67	1.06	Γ_5
icsd_670784	AlCrVZr	216	160.67	1.06	Γ_5
icsd_670799	CaCrPV	216	160.67	0.11	Γ_5
icsd_191684	CoCrTe	216	119.319	0.00	Γ_5
icsd_670707	CoFeGeZr	216	44.231	0.00	Γ_5
icsd_190988	CoMnS	216	119.319	0.00	Γ_5
icsd_053001	CoMnSb	216	160.67	0.00	Γ_5
icsd_190989	CoMnSe	216	119.319	0.00	Γ_5
icsd_190990	CoMnTe	216	119.319	0.00	Γ_5
icsd_053070	CoSbTi	216	44.231	0.00	Γ_5
icsd_053071	CoSbV	216	160.67	0.00	Γ_5
icsd_185079	CoSnV	216	119.319	0.00	Γ_5
icsd_191682	CoTeV	216	119.319	0.00	Γ_5
icsd_191685	CrFeTe	216	44.231	0.00	Γ_5
icsd_670788	CrGaHfV	216	44.231	0.98	Γ_5
icsd_670787	CrGaVZr	216	160.67	1.07	Γ_5
icsd_670793	CrGeScV	216	44.231	0.78	Γ_5
icsd_670796	CrGeVY	216	44.231	0.69	Γ_5
icsd_670791	CrHfInV	216	160.67	0.94	Γ_5
icsd_670790	CrInVZr	216	44.231	1.00	Γ_5
icsd_670798	CrKSV	216	160.67	0.00	Γ_5
icsd_182484	CrNiSb	216	44.231	0.00	Γ_5
icsd_670801	CrPSrV	216	160.67	0.25	Γ_5
icsd_670800	CrRbSV	216	44.231	0.00	Γ_5
icsd_670792	CrScSiV	216	44.231	0.81	Γ_5
icsd_670794	CrScSnV	216	160.67	0.66	Γ_5
icsd_670795	CrSiVY	216	160.67	0.80	Γ_5
icsd_670797	CrSnVY	216	44.231	0.58	Γ_5
icsd_191687	FeMnTe	216	44.231	0.00	Γ_5
icsd_053537	FeSbTi	216	160.67	0.00	Γ_5
icsd_053539	FeSbV	216	119.319	0.00	Γ_5
icsd_106680	FeSnTi	216	160.67	0.00	Γ_5
icsd_191683	FeTeV	216	119.319	0.00	Γ_5
icsd_184947	$GeMn_2$	216	160.67	0.00	Γ_5
icsd_670705	GeMnVZr	216	160.67	0.00	Γ_5
icsd_044660	IrMnSb	216	160.67	0.00	Γ_5
icsd_184948	Mn_2Sb	216	44.231	0.00	Γ_5
icsd_671535	Mn_2Si	216	160.67	0.00	Γ_5
icsd_161714	MnNiP	216	119.319	0.00	Γ_5
icsd_054343	MnRhSb	216	44.231	0.00	Γ_5
icsd_670704	MnSiVZr	216	44.231	0.00	Γ_5
icsd_076702	NiSbV	216	44.231	0.00	Γ_5
icsd_107127	RuSbTi	216	119.319	0.00	Γ_5
icsd_107124	RuSbV	216	119.319	0.02	Γ_5
icsd_043847	$CAlCo_3$	221	123.345	0.00	Γ_4^+
icsd_076790	CCo_3Mg	221	123.345	0.00	Γ_4^+
icsd_076793	CCo_3Sc	221	47.252	0.00	Γ_4^+
icsd_077152	$CMgNi_3$	221	47.252	0.00	Γ_4^+
icsd_077394	CRu_3V	221	123.345	0.00	Γ_4^+
icsd_053506	Fe_3NPd	221	123.345	0.00	Γ_4^+
icsd_044864	Fe_3NPt	221	123.345	0.00	Γ_4^+
icsd_053502	Fe_4N	221	123.345	0.00	Γ_4^+
icsd_044369	Mn_4N	221	123.345	0.00	Γ_4^+
icsd_106087	$SnTi_3$	221	123.345	0.00	Γ_4^+
icsd_057600	$AlCo_2Cr$	225	139.537	0.00	Γ_4^+
icsd_185966	$AlCo_2Ti$	225	139.537	0.00	Γ_4^+
icsd_057643	$AlCo_2V$	225	166.101	0.00	Γ_4^+
icsd_057654	$AlCrFe_2$	225	139.537	0.00	Γ_4^+
icsd_057806	$AlFe_2Mn$	225	71.536	0.00	Γ_4^+
icsd_057807	$AlFe_2Mo$	225	166.101	0.00	Γ_4^+
icsd_057827	$AlFe_2Ti$	225	166.101	0.00	Γ_4^+
icsd_057832	$AlFe_2V$	225	166.101	0.00	Γ_4^+

TABLE S36. Tabulated information on **collinear ferrimagnetic** materials, including the chemical formula, space group, magnetic space group, band gap and corresponding irreducible representations of crystallographic space group.

ICSD number	Chemical formula	SG NUM	BNS	Band Gap (eV)	Irrep
icsd_057994	$AlMn_2V$	225	166.101	0.00	Γ_4^+
icsd_186059	$AsFe_2Ti$	225	166.101	0.00	Γ_4^+
icsd_102318	Co_2CrGa	225	139.537	0.00	Γ_4^+
icsd_416260	Co_2CrIn	225	139.537	0.00	Γ_4^+
icsd_102453	Co_2GaTi	225	139.537	0.00	Γ_4^+
icsd_102456	Co_2GaV	225	166.101	0.00	Γ_4^+
icsd_052989	Co_2GeTi	225	71.536	0.00	Γ_4^+
icsd_053080	Co_2SiTi	225	139.537	0.00	Γ_4^+
icsd_102682	Co_2SnTi	225	139.537	0.00	Γ_4^+
icsd_102684	Co_2SnV	225	166.101	0.00	Γ_4^+
icsd_102437	$CoGa_2Mn$	225	166.101	0.00	Γ_4^+
icsd_102755	$CrFe_2Ga$	225	139.537	0.00	Γ_4^+
icsd_185999	$CrFe_2Sn$	225	71.536	0.00	Γ_4^+
icsd_186721	Fe_2GaMn	225	166.101	0.00	Γ_4^+
icsd_103469	Fe_2GaTi	225	139.537	0.00	Γ_4^+
icsd_103473	Fe_2GaV	225	71.536	0.00	Γ_4^+
icsd_186056	Fe_2InTi	225	166.101	0.00	Γ_4^+
icsd_186060	Fe_2SbTi	225	71.536	0.00	Γ_4^+
icsd_053555	Fe_2SiV	225	166.101	0.00	Γ_4^+
icsd_103641	Fe_2SnTi	225	166.101	0.00	Γ_4^+
icsd_103644	Fe_2SnV	225	166.101	0.00	Γ_4^+
icsd_103813	$GaMn_2V$	225	166.101	0.00	Γ_4^+
icsd_188332	$GaMn_3$	225	166.101	0.00	Γ_4^+
icsd_188334	$GeMn_3$	225	166.101	0.00	Γ_4^+
icsd_671340	$GeRu_2V$	225	166.101	0.00	Γ_4^+
icsd_076227	Mn_3Si	225	166.101	0.00	Γ_4^+
icsd_188333	Mn_3Sn	225	166.101	0.00	Γ_4^+
icsd_671341	Ru_2SbV	225	166.101	0.00	Γ_4^+

D. Noncollinear Ferrimagnetic Materials

The relevant information for noncollinear ferrimagnetic materials is summarized in Table S37-S38, including their chemical formula, space group, magnetic space group, band gap and corresponding irreducible representations of crystallographic space group.

TABLE S37. Tabulated information on **noncollinear ferrimagnetic** materials, including the chemical formula, space group, magnetic space group, band gap and corresponding irreducible representations of crystallographic space group.

ICSD number	Chemical formula	SG NUM	BNS	Band Gap (eV)	Irrep
icsd_065295	$Cs_4Cu_3F_{10}$	2	1.1	3.20	Γ_1^-
icsd_416823	$HCoO_5PZn$	2	2.4	1.69	Γ_1^+
icsd_000902	$AsClCo_2O_4$	11	11.50	3.38	Γ_1^+
icsd_415798	$Cl_2Co_2O_3Te$	11	11.50	2.74	Γ_1^+
icsd_657748	O_2Ti	11	2.4	0.00	Γ_2^+
icsd_088156	Ba_2IrLaO_6	14	14.79	0.50	Γ_2^+
icsd_088158	Ba_2IrLuO_6	14	14.79	0.27	Γ_2^+
icsd_088153	Ba_2IrO_6Sc	14	14.75	0.09	Γ_1^+
icsd_088155	Ba_2IrO_6Y	14	14.79	0.19	Γ_2^+
icsd_152444	Ca_2NiO_6Os	14	14.79	0.12	Γ_2^+
icsd_079495	$CoIrLa_2O_6$	14	14.75	0.45	Γ_1^+
icsd_030410	CuO_6Sb_2	14	14.79	1.28	Γ_2^+
icsd_165398	F_4Ru	14	14.75	1.55	Γ_1^+
icsd_006044	F_6Li_2Rh	14	14.75	0.47	Γ_1^+
icsd_195628	$FeMn_2O_6Re$	14	14.75	0.00	Γ_1^+
icsd_238316	InO_6OsSr_2	14	14.79	1.02	Γ_2^+
icsd_414605	$IrLa_2LiO_6$	14	14.79	0.36	Γ_2^+
icsd_079492	$IrLa_2MgO_6$	14	14.79	0.59	Γ_2^+
icsd_413634	$IrLa_2NaO_6$	14	14.79	0.47	Γ_2^+
icsd_079494	$IrLa_2NiO_6$	14	14.75	0.52	Γ_1^+
icsd_075596	$IrLa_2O_6Zn$	14	14.79	0.50	Γ_2^+
icsd_088157	$IrLuO_6Sr_2$	14	14.79	0.24	Γ_2^+
icsd_088152	IrO_6ScSr_2	14	14.79	0.02	Γ_2^+
icsd_088154	IrO_6Sr_2Y	14	14.79	0.26	Γ_2^+
icsd_416199	La_2LiO_6Os	14	14.79	1.00	Γ_2^+
icsd_088522	La_2MgO_6Rh	14	14.75	0.00	Γ_1^+
icsd_088523	La_2O_6RhZn	14	14.79	0.09	Γ_2^+
icsd_159030	$CaIrO_3$	36	36.174	0.34	Γ_4
icsd_429116	$BRuTa$	51	51.295	0.00	Γ_3^+
icsd_263013	Fe_3O_4	51	51.295	0.00	Γ_3^+
icsd_612536	B_2BaNi_2	58	58.398	0.00	Γ_3^+
icsd_615019	B_2Ni_2Sr	58	14.75	0.00	Γ_4^+
icsd_406953	$AsCoHf$	62	62.446	0.00	Γ_2^+
icsd_193272	Bi_3Co	62	62.447	0.00	Γ_3^+
icsd_245840	$CaCrO_3$	62	62.448	0.40	Γ_4^+
icsd_159433	$CaIrO_3$	62	62.448	0.15	Γ_4^+
icsd_167128	$CCoFe_2$	62	62.447	0.00	Γ_3^+
icsd_670824	CCr_2Fe	62	62.446	0.00	Γ_2^+
icsd_181711	CCr_3	62	62.446	0.00	Γ_2^+
icsd_670838	$CFeV_2$	62	62.446	0.00	Γ_2^+
icsd_251180	CMn_3	62	62.446	0.00	Γ_2^+
icsd_625259	Co_3Sn_2	62	62.447	0.00	Γ_3^+
icsd_636746	$GeIrTi$	62	62.446	0.00	Γ_2^+
icsd_196446	IrO_3Sr	62	62.448	0.07	Γ_4^+
icsd_075569	LaO_3Ru	62	62.447	0.61	Γ_3^+
icsd_056697	O_3RuSr	62	62.447	0.00	Γ_3^+
icsd_236435	CoO_6OsSr_2	87	12.62	0.04	$\Gamma_3^+\Gamma_4^+$
icsd_245819	CuO_6OsSr_2	87	12.62	0.00	$\Gamma_3^+\Gamma_4^+$
icsd_024563	S_4V_5	87	12.62	0.00	$\Gamma_3^+\Gamma_4^+$
icsd_652166	Se_4V_5	87	12.62	0.33	$\Gamma_3^+\Gamma_4^+$
icsd_023173	F_6Li_2Mo	94	18.19	1.13	Γ_5
icsd_025751	Cr_3GeN	113	18.19	0.00	Γ_5
icsd_030447	BCo_2	121	72.544	0.00	Γ_5
icsd_160691	CCr_2LaSi_2	123	65.486	0.00	Γ_5^+
icsd_187494	$FeGaNi_2$	123	12.58	0.00	Γ_5^+
icsd_187493	$GaMnNi_2$	123	12.58	0.00	Γ_5^+
icsd_021110	CuF_3K	127	55.358	2.49	Γ_5^+
icsd_611100	As_2Ni_4Y	136	65.486	0.00	Γ_5^+
icsd_166673	CoO_6Ta_2	136	58.398	3.01	Γ_5^+
icsd_418676	CrF_6Li_2	136	58.398	1.01	Γ_5^+
icsd_424578	Cs_3NiO_2	136	58.398	1.58	Γ_5^+
icsd_084789	CuO_6Sb_2	136	58.398	1.30	Γ_5^+
icsd_074565	F_6Li_2Mo	136	58.398	1.20	Γ_5^+
icsd_095778	F_6Li_2Rh	136	58.398	0.47	Γ_5^+
icsd_040337	FeO_6Ta_2	136	58.398	2.36	Γ_5^+

TABLE S38. Tabulated information on **noncollinear ferrimagnetic** materials, including the chemical formula, space group, magnetic space group, band gap and corresponding irreducible representations of crystallographic space group.

ICSD number	Chemical formula	SG NUM	BNS	Band Gap (eV)	Irrep
icsd_262579	K_3NiO_2	136	58.398	1.58	Γ_5^+
icsd_424579	NiO_2Rb_3	136	58.398	1.31	Γ_5^+
icsd_025775	$CGeMn_3$	140	72.544	0.00	Γ_5^+
icsd_024651	Fe_2N	149	162.77	0.00	Γ_2
icsd_200999	Li_2O_3Re	161	9.37	0.37	Γ_3
icsd_044612	Fe_2N	162	162.77	0.00	Γ_2^+
icsd_041814	Sb_2V_3	166	12.58	0.00	Γ_3^+
icsd_016673	F_3Ru	167	15.85	1.39	Γ_3^+
icsd_016649	F_3Ti	167	15.85	2.19	Γ_3^+
icsd_030624	F_3V	167	15.85	2.03	Γ_3^+
icsd_088670	$BaCoO_3$	187	38.191	1.35	Γ_6
icsd_624869	$Co_2S_6Ta_9$	189	38.189	0.00	Γ_6
icsd_623085	CoGaHf	189	38.189	0.00	Γ_6
icsd_623254	CoGaZr	189	38.191	0.00	Γ_6
icsd_626107	Cr_6Ge_6Sc	191	191.239	0.00	Γ_3^+
icsd_658018	Cr_6Ge_6Y	191	191.239	0.00	Γ_3^+
icsd_029285	NP_3V_5	193	193.258	0.00	Γ_4^+
icsd_016839	CoSi	198	19.27	0.00	Γ_4
icsd_166458	N_2Os	205	61.436	0.00	Γ_4^+
icsd_635637	Ga_2V_3	213	155.45	0.00	Γ_5
icsd_052592	$AgMn_3N$	221	166.97	0.00	Γ_5^+
icsd_058547	$AuNV_3$	221	12.58	0.00	Γ_5^+
icsd_043853	$CAlFe_3$	221	12.62	0.00	Γ_4^+
icsd_043860	$CAlMn_3$	221	12.58	0.00	Γ_5^+
icsd_076842	CFe_3Sn	221	166.101	0.00	Γ_4^+
icsd_076763	CFe_3Zn	221	65.486	0.00	Γ_4^+
icsd_023586	$CGaMn_3$	221	12.62	0.00	Γ_4^+
icsd_044351	$CGeMn_3$	221	12.58	0.00	Γ_5^+
icsd_077036	$CInMn_3$	221	12.62	0.00	Γ_4^+
icsd_077153	CMn_3Sn	221	12.58	0.00	Γ_5^+
icsd_247066	Co_3InN	221	10.46	0.00	Γ_4^+
icsd_053125	Cr_3GaN	221	166.97	0.00	Γ_5^+
icsd_053132	Cr_3IrN	221	166.101	0.00	Γ_4^+
icsd_053143	Cr_3NRh	221	166.101	0.00	Γ_4^+
icsd_053145	Cr_3NSn	221	12.58	0.00	Γ_5^+
icsd_053306	$CuMn_3N$	221	166.97	0.00	Γ_5^+
icsd_183372	$CuNNi_3$	221	65.486	0.00	Γ_4^+
icsd_044865	Fe_3NNi	221	166.101	0.00	Γ_4^+
icsd_153274	Fe_3NRh	221	12.62	0.00	Γ_4^+
icsd_087399	$GaMn_3N$	221	12.58	0.00	Γ_5^+
icsd_097743	$GeMn_3$	221	166.101	0.00	Γ_4^+
icsd_044659	$IrMn_3N$	221	65.486	0.00	Γ_4^+
icsd_076056	Mn_3NNi	221	166.101	0.00	Γ_4^+
icsd_076057	Mn_3NPd	221	166.101	0.00	Γ_4^+
icsd_076058	Mn_3NPt	221	166.101	0.00	Γ_4^+
icsd_076060	Mn_3NRh	221	166.101	0.00	Γ_4^+
icsd_076062	Mn_3NSn	221	166.101	0.00	Γ_4^+
icsd_076070	Mn_3NZn	221	166.97	0.00	Γ_5^+
icsd_096119	Mn_3Sb	221	166.101	0.00	Γ_4^+
icsd_076403	NNi_4	221	166.97	0.00	Γ_5^+

E. Collinear Antiferromagnetic Materials

The relevant information for collinear antiferromagnetic materials is summarized in Table S39-S48, including their chemical formula, space group, magnetic space group, band gap and corresponding irreducible representations of crystallographic space group.

TABLE S39. Tabulated information on **collinear antiferromagnetic** materials, including the chemical formula, space group, magnetic space group, band gap and corresponding irreducible representations of crystallographic space group.

ICSD number	Chemical formula	SG NUM	BNS	Band Gap (eV)	Irrep
icsd_100442	$As_2Fe_4O_{11}$	2	2.6	2.34	Γ_1^-
icsd_428633	$AsBiCoO_5$	2	2.6	3.03	Γ_1^-
icsd_059721	$AsBiMnO_5$	2	2.6	2.71	Γ_1^-
icsd_092916	$AsBiNiO_5$	2	2.6	3.16	Γ_1^-
icsd_043508	AsFeS	2	2.6	0.00	Γ_1^-
icsd_024284	$B_2Co_2O_5$	2	2.6	3.62	Γ_1^-
icsd_246811	$B_2Fe_2O_5$	2	2.6	3.24	Γ_1^-
icsd_006240	Ba_2CuO_6Te	2	2.6	1.41	Γ_1^-
icsd_059720	$BiMnO_5V$	2	2.6	2.48	Γ_1^-
icsd_418858	$Br_2CoO_3Sb_2$	2	2.6	2.62	Γ_1^-
icsd_039784	Br_3Ti	2	2.6	2.27	Γ_1^-
icsd_410101	Cl_7MoOSe	2	2.6	1.78	Γ_1^-
icsd_196024	$CMnO_3$	2	2.6	3.01	Γ_1^-
icsd_423336	Cs_4FeO_3	2	2.6	1.37	Γ_1^-
icsd_240930	$Cu_2Na_2O_{11}Si_4$	2	2.6	2.90	Γ_1^-
icsd_039439	$CuMoO_4$	2	2.6	2.02	Γ_1^-
icsd_004189	CuO_4W	2	2.6	1.94	Γ_1^-
icsd_173748	$F_2O_7Te_2V_2$	2	2.6	2.67	Γ_1^-
icsd_036208	$Fe_2O_7P_2$	2	2.6	3.83	Γ_1^-
icsd_196300	FeSe	2	2.6	1.21	Γ_1^-
icsd_180390	$FFeO_4S$	2	2.4	2.30	Γ_1^+
icsd_180391	$FLiNiO_4S$	2	2.4	3.71	Γ_1^+
icsd_087710	H_2FeO_5V	2	2.6	2.49	Γ_1^-
icsd_167608	$HFeLiO_5P$	2	2.4	2.64	Γ_1^+
icsd_095571	$LiMoS_2$	2	2.6	0.56	Γ_1^-
icsd_023334	MnP_4	2	2.6	0.00	Γ_1^-
icsd_166313	NaO_6Si_2Ti	2	2.6	2.78	Γ_1^-
icsd_036263	MoO_2	4	4.9	0.00	Γ_2
icsd_069869	$CaClFeO_2$	8	8.32	1.96	Γ_1
icsd_055578	$Co_2In_5Zr_4$	10	10.44	0.00	Γ_2^-
icsd_081569	$Fe_2O_{12}Se_4Sr$	10	10.42	2.33	Γ_1^+
icsd_601978	H_2FeTi	10	10.45	0.00	Γ_1^-
icsd_000901	$AsClCu_2O_4$	11	11.54	1.38	Γ_2^+
icsd_162834	$BiFeO_3$	11	11.55	0.00	Γ_2^-
icsd_411140	Cl_7CsTi_2	11	11.52	2.68	Γ_2^-
icsd_065346	$ClFeLiMoO_4$	11	11.52	2.67	Γ_2^-
icsd_001029	CoI_4Rb_2	11	11.53	2.05	Γ_1^-
icsd_108896	CoO_3Sr	11	11.50	0.00	Γ_1^+
icsd_084825	$CoPZr_2$	11	11.53	0.00	Γ_1^-
icsd_035044	$Cr_2Nb_2Se_{10}$	11	11.52	0.00	Γ_2^-
icsd_166587	CsF_5NOOs	11	11.53	1.68	Γ_1^-
icsd_422751	$CuNa_2O_2$	11	11.53	1.33	Γ_1^-
icsd_166586	F_5KNOOs	11	11.53	1.63	Γ_1^-
icsd_078042	$F_7MnRbZr$	11	11.53	4.76	Γ_1^-
icsd_078041	$F_7MnTlZr$	11	11.52	3.77	Γ_2^-
icsd_066513	$FeTaTe_3$	11	11.52	0.00	Γ_2^-
icsd_187148	H_4Fe	11	11.53	0.00	Γ_1^-
icsd_075454	$As_2Ba_2Mn_2O$	12	12.61	1.02	Γ_1^-
icsd_043898	As_2Cr	12	12.60	0.00	Γ_2^-
icsd_611574	As_2V	12	12.60	0.00	Γ_2^-
icsd_195677	$BiBrFeS_2$	12	12.58	1.46	Γ_1^+
icsd_415307	$BiBrMnS_2$	12	12.62	1.33	Γ_2^+
icsd_415138	$BiIMnSe_2$	12	12.62	0.92	Γ_2^+
icsd_423461	Br_4W	12	12.60	0.25	Γ_2^-
icsd_172782	$BrMnS_2Sb$	12	12.62	1.40	Γ_2^+
icsd_072389	Ca_2FeN_2	12	12.61	0.94	Γ_1^-
icsd_096556	$CaClFeO_2$	12	12.60	2.10	Γ_2^-
icsd_617825	$CFe_2Si_2Y_2$	12	12.61	0.00	Γ_1^-
icsd_041802	Cl_3CrCs	12	12.62	1.02	Γ_2^+
icsd_002225	Cl_3CrRb	12	12.62	1.21	Γ_2^+
icsd_026108	Cl_3Mo	12	12.61	2.37	Γ_1^-
icsd_262639	Cl_3Tc	12	12.60	1.16	Γ_2^-
icsd_624616	$Co_2P_2S_6$	12	12.60	1.91	Γ_2^-
icsd_290048	Fe_2LuO_4	12	12.61	0.00	Γ_1^-
icsd_016252	$Fe_2P_2S_6$	12	12.61	2.12	Γ_1^-

TABLE S40. Tabulated information on **collinear antiferromagnetic** materials, including the chemical formula, space group, magnetic space group, band gap and corresponding irreducible representations of crystallographic space group.

ICSD number	Chemical formula	SG NUM	BNS	Band Gap (eV)	Irrep
icsd_061392	$FePS_3$	12	12.61	2.10	Γ_1^-
icsd_030011	FeS_2Tl	12	12.61	1.19	Γ_1^-
icsd_020661	$FeSc_2Si_2$	12	12.61	0.00	Γ_1^-
icsd_100354	$FeSe_2Tl$	12	12.60	0.80	Γ_2^-
icsd_671146	H_3MgNi_2	12	12.61	0.00	Γ_1^-
icsd_281558	$IMnSbSe_2$	12	12.62	0.89	Γ_2^+
icsd_049021	$KLiMnO_2$	12	12.60	1.43	Γ_2^-
icsd_061391	$MnPS_3$	12	12.61	2.26	Γ_1^-
icsd_657314	$Ni_2P_2S_6$	12	12.61	1.70	Γ_1^-
icsd_602341	$NiPS_3$	12	12.61	1.72	Γ_1^-
icsd_646145	$NiPSe_3$	12	12.60	1.29	Γ_2^-
icsd_647926	$P_2Pd_2S_6$	12	12.61	0.41	Γ_1^-
icsd_648076	$P_2S_6V_2$	12	12.61	2.15	Γ_1^-
icsd_036456	$Ag_{0.5}Cr_{0.5}PS_3$	13	13.68	1.31	Γ_1^-
icsd_202045	$Ag_{0.5}PS_3V_{0.5}$	13	13.68	0.88	Γ_1^-
icsd_186505	AsCaFFe	13	13.67	0.00	Γ_2^-
icsd_186508	AsFFeSr	13	13.67	0.00	Γ_2^-
icsd_010293	Cl_4Re	13	13.68	0.80	Γ_1^-
icsd_067168	Cl_7CsTi_2	13	13.67	2.77	Γ_2^-
icsd_063686	ClF_6O_2Ru	13	13.68	0.79	Γ_1^-
icsd_081061	$CoMoO_4$	13	13.68	2.37	Γ_1^-
icsd_015851	CoO_4W	13	13.67	3.01	Γ_2^-
icsd_008128	$FeNbO_4$	13	13.67	2.39	Γ_2^-
icsd_015192	FeO_4W	13	13.68	1.29	Γ_1^-
icsd_411172	$K_2Mn_3S_4$	13	13.67	2.62	Γ_2^-
icsd_061078	$MnMoO_4$	13	13.67	1.95	Γ_2^-
icsd_015850	MnO_4W	13	13.68	2.66	Γ_1^-
icsd_081060	$MoNiO_4$	13	13.67	2.26	Γ_2^-
icsd_015852	NiO_4W	13	13.67	2.70	Γ_2^-
icsd_185809	AsFeS	14	14.77	0.00	Γ_2^-
icsd_610526	AsFeSe	14	14.77	0.00	Γ_2^-
icsd_610529	AsFeTe	14	14.78	0.00	Γ_1^-
icsd_054136	Br_3CrIn	14	14.78	1.28	Γ_1^-
icsd_190486	Ca_2InO_6Os	14	14.75	0.89	Γ_1^+
icsd_291608	Ca_2O_6OsSc	14	14.75	0.70	Γ_1^+
icsd_015590	Cl_3CuK	14	14.77	1.64	Γ_2^-
icsd_239557	Cl_3CuTl	14	14.77	1.10	Γ_2^-
icsd_004411	Cl_3MoO	14	14.77	1.81	Γ_2^-
icsd_074940	CoK_2O_2	14	14.77	2.38	Γ_2^-
icsd_073739	$CoNbTe_2$	14	14.78	0.00	Γ_1^-
icsd_073738	$CoTaTe_2$	14	14.78	0.00	Γ_1^-
icsd_009390	CrO_6Ta_2	14	14.79	0.00	Γ_2^+
icsd_202451	CuO_3Te	14	14.77	1.78	Γ_2^-
icsd_633086	FePS	14	14.77	0.00	Γ_2^-
icsd_633093	FePSe	14	14.77	0.00	Γ_2^-
icsd_633399	FeSbSe	14	14.77	0.00	Γ_2^-
icsd_633405	FeSbTe	14	14.77	0.00	Γ_2^-
icsd_038384	HClCuO	14	14.77	1.81	Γ_2^-
icsd_084949	$HMnO_2$	14	14.77	1.76	Γ_2^-
icsd_061038	$K_2Mn_2O_3$	14	14.78	1.47	Γ_1^-
icsd_023722	MoO_2	14	14.77	0.00	Γ_2^-
icsd_173152	O_2Tc	14	14.77	0.30	Γ_2^-
icsd_015889	O_2V	14	14.77	1.47	Γ_2^-
icsd_002790	CrP_4	15	15.87	0.00	Γ_2^-
icsd_015557	$FeKS_2$	15	15.88	1.45	Γ_1^-
icsd_040780	$FeKSe_2$	15	15.88	1.06	Γ_1^-
icsd_202381	$FeRbS_2$	15	15.88	1.50	Γ_1^-
icsd_040781	$FeRbSe_2$	15	15.87	1.10	Γ_2^-
icsd_006286	O_3V_2	15	15.88	1.34	Γ_1^-
icsd_038315	P_4V	15	15.87	0.00	Γ_2^-
icsd_037026	$FeNaS_2$	23	23.51	1.65	Γ_2
icsd_081204	Ca_2FeO_6W	25	25.59	0.53	Γ_4
icsd_015105	$LiMnO_2$	25	59.407	1.90	Γ_3
icsd_040044	CoSSb	31	31.127	0.00	Γ_2
icsd_081167	$Ba_2Cu_3LaO_7$	47	47.253	0.00	Γ_1^-

TABLE S41. Tabulated information on **collinear antiferromagnetic** materials, including the chemical formula, space group, magnetic space group, band gap and corresponding irreducible representations of crystallographic space group.

ICSD number	Chemical formula	SG NUM	BNS	Band Gap (eV)	Irrep
icsd_161972	$Ba_2Cu_3LuO_7$	47	47.253	0.00	Γ_1^-
icsd_041646	$Ba_2Cu_3O_7Y$	47	47.253	0.00	Γ_1^-
icsd_171433	$BaCo_2O_5Y$	47	47.251	0.00	Γ_4^-
icsd_164175	$BaFe_2O_5Y$	51	51.291	0.62	Γ_3^-
icsd_035130	$Ca_2Mn_2O_5$	55	55.356	1.20	Γ_2^-
icsd_035219	$CaMnO_{2.5}$	55	55.356	0.90	Γ_2^-
icsd_073399	$Cu_2La_2O_5$	55	55.359	0.69	Γ_1^-
icsd_077943	$CuLaO_{2.5}$	55	55.359	0.69	Γ_1^-
icsd_090183	$Mn_2O_5Sr_2$	55	55.356	0.82	Γ_2^-
icsd_670573	CFe_2	57	57.385	0.00	Γ_1^-
icsd_020933	Fe_2HfSi_2	57	57.380	0.00	Γ_4^-
icsd_087157	Fe_2ScSi_2	57	57.381	0.00	Γ_2^-
icsd_016895	CCo_2	58	58.396	0.00	Γ_2^-
icsd_076826	CFe_2	58	58.395	0.00	Γ_3^-
icsd_016894	Co_2N	58	58.399	0.00	Γ_1^-
icsd_165626	$BaCrS_2$	59	59.407	0.17	Γ_4^-
icsd_428170	$BaFe_2OS_2$	59	59.411	2.47	Γ_1^-
icsd_009422	Br_3Mo	59	59.407	2.00	Γ_3^-
icsd_028119	Br_3Ru	59	59.411	0.47	Γ_1^-
icsd_260162	Br_3Tc	59	59.407	0.59	Γ_3^-
icsd_080372	C_2CrSc	59	59.407	0.00	Γ_3^-
icsd_015094	$CaCu_2O_3$	59	59.410	0.57	Γ_3^+
icsd_414041	Cl_3Ru	59	59.411	0.38	Γ_1^-
icsd_016013	ClFeO	59	59.407	1.48	Γ_3^-
icsd_025657	ClOTi	59	59.411	2.49	Γ_1^-
icsd_053146	CrN	59	59.407	0.00	Γ_3^-
icsd_195025	Fe_2OS_2Sr	59	59.411	2.47	Γ_1^-
icsd_195027	Fe_2OSe_2Sr	59	59.411	2.36	Γ_1^-
icsd_173784	I_3Ti	59	59.407	1.51	Γ_4^-
icsd_074648	I_3Zr	59	59.407	0.63	Γ_3^-
icsd_015768	$LiMnO_2$	59	59.407	1.40	Γ_4^-
icsd_015769	$MnNaO_2$	59	59.407	1.64	Γ_4^-
icsd_646747	Ni_3Sn	59	59.411	0.00	Γ_1^-
icsd_009965	CV_2	60	60.420	0.00	Γ_4^-
icsd_042979	Mn_2N	60	60.425	0.00	Γ_1^-
icsd_048026	AsCo	62	62.449	0.00	Γ_1^-
icsd_610084	AsCoMn	62	62.444	0.00	Γ_4^-
icsd_043896	AsCoRh	62	62.444	0.00	Γ_4^-
icsd_023589	AsCr	62	62.443	0.00	Γ_3^-
icsd_072413	AsCuMn	62	62.444	0.05	Γ_4^-
icsd_030413	AsFe	62	62.444	0.00	Γ_4^-
icsd_610502	AsFeNb	62	62.449	0.00	Γ_1^-
icsd_610528	AsFeTa	62	62.443	0.00	Γ_3^-
icsd_611086	AsNiTi	62	62.443	0.00	Γ_3^-
icsd_611097	AsNiV	62	62.443	0.00	Γ_3^-
icsd_044052	AsRhTi	62	62.445	0.00	Γ_2^-
icsd_107965	AsRhV	62	62.443	0.11	Γ_3^-
icsd_042577	AsRu	62	62.444	0.00	Γ_4^-
icsd_042446	AsV	62	62.449	0.00	Γ_1^-
icsd_425310	B_2Fe	62	62.443	0.30	Γ_3^-
icsd_031453	$BaMnS_2$	62	62.449	2.03	Γ_1^-
icsd_030450	BCo	62	62.449	0.00	Γ_1^-
icsd_020461	BCoMo	62	62.443	0.00	Γ_3^-
icsd_020079	BCoRe	62	62.441	0.00	Γ_1^+
icsd_613388	BCoW	62	62.443	0.00	Γ_3^-
icsd_614256	BFeW	62	62.446	0.00	Γ_2^+
icsd_172156	$BiClMnS_2$	62	62.444	1.63	Γ_4^-
icsd_247467	$BiCoO_3$	62	62.446	1.00	Γ_2^+
icsd_160454	$BiCrO_3$	62	62.446	1.61	Γ_2^+
icsd_076630	BMn	62	62.443	0.00	Γ_3^-
icsd_075469	Br_3FeIn	62	62.443	1.83	Γ_3^-
icsd_036217	Br_3FeTl	62	62.443	2.36	Γ_3^-
icsd_172784	$BrMnSbSe_2$	62	62.444	1.29	Γ_4^-
icsd_238684	CaFeOSe	62	62.444	2.20	Γ_4^-
icsd_670821	$CAlFe_2$	62	62.449	0.00	Γ_1^-

TABLE S42. Tabulated information on **collinear antiferromagnetic** materials, including the chemical formula, space group, magnetic space group, band gap and corresponding irreducible representations of crystallographic space group.

ICSD number	Chemical formula	SG NUM	BNS	Band Gap (eV)	Irrep
icsd_153239	$CaMnO_{2.98}$	62	62.448	0.53	Γ_4^+
icsd_052705	$CaMnSb_2$	62	62.449	0.01	Γ_1^-
icsd_261341	CaO_3Tc	62	62.448	1.50	Γ_4^+
icsd_043521	CCo_3	62	62.444	0.00	Γ_4^-
icsd_670826	CCu_2Fe	62	62.449	0.00	Γ_1^-
icsd_670834	CFe_2Ta	62	62.448	0.00	Γ_4^+
icsd_670836	CFe_2Ti	62	62.444	0.00	Γ_4^-
icsd_670839	CFe_2W	62	62.448	0.00	Γ_4^+
icsd_016593	CFe_3	62	62.444	0.00	Γ_4^-
icsd_670829	$CFeMo_2$	62	62.449	0.00	Γ_1^-
icsd_670835	$CFeTa_2$	62	62.449	0.00	Γ_1^-
icsd_670840	$CFeW_2$	62	62.449	0.00	Γ_1^-
icsd_004063	Cl_3FeK	62	62.449	3.71	Γ_1^-
icsd_151925	$ClMnS_2Sb$	62	62.444	1.66	Γ_4^-
icsd_623417	Co_2Ge	62	62.449	0.00	Γ_1^-
icsd_044858	Co_2Si	62	62.449	0.00	Γ_1^-
icsd_165248	CoCrSi	62	62.449	0.00	Γ_1^-
icsd_004404	CoF_3Na	62	62.448	4.25	Γ_4^+
icsd_165250	CoFeSi	62	62.449	0.00	Γ_1^-
icsd_623231	CoGaY	62	62.447	0.00	Γ_3^+
icsd_623439	CoGeHf	62	62.449	0.00	Γ_1^-
icsd_623540	CoGeNb	62	62.445	0.00	Γ_2^-
icsd_428472	CoGeSc	62	62.445	0.00	Γ_2^-
icsd_623611	CoGeTa	62	62.444	0.00	Γ_4^-
icsd_623660	CoGeV	62	62.444	0.00	Γ_4^-
icsd_601866	CoGeY	62	62.446	0.00	Γ_2^+
icsd_623685	CoGeZr	62	62.449	0.00	Γ_1^-
icsd_623786	CoHfP	62	62.443	0.00	Γ_3^-
icsd_172052	$CoLuO_3$	62	62.448	1.74	Γ_4^+
icsd_601862	CoLuSn	62	62.449	0.00	Γ_1^-
icsd_624322	CoNbSi	62	62.449	0.00	Γ_1^-
icsd_624659	CoPV	62	62.449	0.00	Γ_1^-
icsd_624977	CoScSn	62	62.446	0.00	Γ_2^+
icsd_625050	CoSiTa	62	62.449	0.00	Γ_1^-
icsd_053079	CoSiTi	62	62.445	0.00	Γ_2^-
icsd_165247	CoSiV	62	62.449	0.00	Γ_1^-
icsd_601850	CoSnY	62	62.447	0.00	Γ_3^+
icsd_151867	CrFeP	62	62.444	0.00	Γ_4^-
icsd_626157	CrHfSi	62	62.449	0.00	Γ_1^-
icsd_626229	$CrLaSe_3$	62	62.443	0.41	Γ_3^-
icsd_251093	$CrLuO_3$	62	62.446	2.53	Γ_2^+
icsd_053189	CrNbP	62	62.443	0.00	Γ_3^-
icsd_109352	CrO_3Y	62	62.446	2.43	Γ_2^+
icsd_005418	CrP	62	62.443	0.00	Γ_3^-
icsd_626529	CrPZr	62	62.444	0.00	Γ_4^-
icsd_626850	CrSiZr	62	62.444	0.00	Γ_4^-
icsd_093161	CrTe	62	62.443	0.00	Γ_3^-
icsd_670816	CTi_3	62	59.407	0.00	Γ_4^-
icsd_071221	Cu_2LiO_2	62	62.444	1.33	Γ_4^-
icsd_067558	Cu_2NaO_2	62	62.444	1.36	Γ_4^-
icsd_072411	CuMnP	62	62.443	0.31	Γ_3^-
icsd_670817	CV_3	62	62.450	0.00	Γ_3^-
icsd_006047	F_3KPd	62	74.562	2.35	Γ_4^+
icsd_260758	Fe_3N	62	62.449	0.00	Γ_1^-
icsd_632129	FeGeTa	62	62.446	0.00	Γ_2^+
icsd_632166	FeGeZr	62	62.443	0.00	Γ_3^-
icsd_086280	FeHfP	62	62.443	0.00	Γ_3^-
icsd_632263	FeHfSi	62	62.445	0.00	Γ_2^-
icsd_026422	FeI_3Tl	62	62.443	1.80	Γ_3^-
icsd_632538	FeMnP	62	62.449	0.00	Γ_1^-
icsd_632646	FeMoP	62	62.444	0.00	Γ_4^-
icsd_632827	FeNbSi	62	62.445	0.00	Γ_2^-
icsd_246514	FeO_3Ti	62	62.445	1.88	Γ_2^-
icsd_043248	FeP	62	62.444	0.00	Γ_4^-
icsd_049729	FePTa	62	62.443	0.00	Γ_3^-

TABLE S43. Tabulated information on **collinear antiferromagnetic** materials, including the chemical formula, space group, magnetic space group, band gap and corresponding irreducible representations of crystallographic space group.

ICSD number	Chemical formula	SG NUM	BNS	Band Gap (eV)	Irrep
icsd_633111	FePTi	62	62.449	0.00	Γ_1^-
icsd_633116	FePV	62	62.443	0.00	Γ_3^-
icsd_035008	FeS	62	62.446	1.05	Γ_2^+
icsd_076346	FeScSi	62	62.445	0.00	Γ_2^-
icsd_633568	FeSiTa	62	62.443	0.00	Γ_3^-
icsd_633674	FeSiZr	62	62.444	0.00	Γ_4^-
icsd_097805	GeMnY	62	62.444	0.00	Γ_4^-
icsd_053716	GeMnZr	62	62.449	0.00	Γ_1^-
icsd_637435	GeNiV	62	62.444	0.00	Γ_4^-
icsd_409926	GePdTi	62	62.449	0.04	Γ_1^-
icsd_239321	$HFeO_2$	62	62.444	2.20	Γ_4^-
icsd_053024	HfMnSi	62	62.444	0.00	Γ_4^-
icsd_656389	HfPV	62	62.444	0.00	Γ_4^-
icsd_083987	LuMnSi	62	62.444	0.00	Γ_4^-
icsd_643093	MnNiP	62	62.449	0.00	Γ_1^-
icsd_030412	MnP	62	62.445	0.00	Γ_2^-
icsd_085947	MnPTa	62	62.446	0.00	Γ_2^+
icsd_238591	MnS	62	62.449	0.00	Γ_1^-
icsd_643539	$MnSb_2Sr$	62	62.449	0.05	Γ_1^-
icsd_076236	MnSiZr	62	62.444	0.00	Γ_4^-
icsd_076241	MnTe	62	62.449	0.00	Γ_1^-
icsd_091273	N_2NiSr_2	62	62.444	0.43	Γ_4^-
icsd_252431	NaO_3Os	62	62.448	0.35	Γ_4^+
icsd_645178	NbPV	62	62.444	0.00	Γ_4^-
icsd_646176	NiPV	62	62.443	0.00	Γ_3^-
icsd_165254	NiSiV	62	62.449	0.00	Γ_1^-
icsd_648877	PdSiTi	62	62.445	0.00	Γ_2^-
icsd_109139	PRu	62	62.444	0.00	Γ_4^-
icsd_260794	PtSiTi	62	62.445	0.06	Γ_2^-
icsd_077856	PV_2	62	62.445	0.00	Γ_2^-
icsd_039562	PVZr	62	62.444	0.00	Γ_4^-
icsd_000990	RuSb	62	62.444	0.00	Γ_4^-
icsd_652036	SeTi	62	62.449	0.00	Γ_1^-
icsd_043494	SiTi	62	62.445	0.00	Γ_2^-
icsd_024564	SV	62	62.449	1.68	Γ_1^-
icsd_670675	$AlTi_2Zr$	63	63.465	0.00	Γ_1^-
icsd_195899	$AsCo_2LaN$	63	63.461	0.00	Γ_2^-
icsd_195898	$AsFe_2LaN$	63	63.465	0.00	Γ_1^-
icsd_195900	$AsLaNNi_2$	63	63.460	0.00	Γ_4^-
icsd_610970	$AsNV_3$	63	63.459	0.00	Γ_3^-
icsd_601350	B_3Cr_2	63	63.461	0.00	Γ_2^-
icsd_079258	B_3V_2	63	63.465	0.00	Γ_1^-
icsd_252147	BaCoOS	63	63.459	2.35	Γ_3^-
icsd_030603	BCr	63	63.461	0.00	Γ_2^-
icsd_613898	BFe	63	63.459	0.00	Γ_3^-
icsd_042952	BV	63	63.465	0.00	Γ_1^-
icsd_020297	C_2Cr_2V	63	63.465	0.00	Γ_1^-
icsd_025524	$CaIrO_3$	63	63.464	0.29	Γ_4^+
icsd_025761	$CAsV_3$	63	63.465	0.00	Γ_1^-
icsd_617981	$CGeV_3$	63	63.459	0.00	Γ_3^-
icsd_618621	CPV_3	63	63.461	0.00	Γ_2^-
icsd_632049	$FeGe_2La$	63	63.461	0.00	Γ_2^-
icsd_632434	$FeLaSi_2$	63	63.459	0.00	Γ_3^-
icsd_187134	FeLiP	63	63.459	0.00	Γ_3^-
icsd_246516	FeO_3Ti	63	63.459	1.56	Γ_3^-
icsd_634723	$GaNV_3$	63	63.461	0.00	Γ_2^-
icsd_637164	$GeNV_3$	63	63.465	0.00	Γ_1^-
icsd_024885	$HFeO_2$	63	63.459	1.69	Γ_3^-
icsd_085926	$LaMnSi_2$	63	63.465	0.00	Γ_1^-
icsd_189761	$SnTi_3$	63	63.459	0.00	Γ_3^-
icsd_099041	Cu_2O_3Sr	65	65.483	0.52	Γ_3^-
icsd_174209	F_7KTi_2	65	65.487	2.51	Γ_1^-
icsd_261512	$Fe_2O_5Sr_3$	65	65.484	0.00	Γ_2^-
icsd_009389	OTi_2Zr	65	65.483	0.00	Γ_3^-
icsd_186504	AsCaFFe	67	67.503	0.00	Γ_3^-

TABLE S44. Tabulated information on **collinear antiferromagnetic** materials, including the chemical formula, space group, magnetic space group, band gap and corresponding irreducible representations of crystallographic space group.

ICSD number	Chemical formula	SG NUM	BNS	Band Gap (eV)	Irrep
icsd_180434	AsFeLaO	67	67.503	0.00	Γ_4^-
icsd_168206	AsFeLi	67	67.503	0.00	Γ_4^-
icsd_163916	AsFFeSr	67	67.503	0.00	Γ_3^-
icsd_075515	$BaCoS_2$	67	67.503	0.24	Γ_3^-
icsd_163555	FeSe	67	67.503	1.22	Γ_4^-
icsd_166020	As_2BaFe_2	69	69.523	0.00	Γ_3^-
icsd_166017	As_2CaFe_2	69	69.523	0.00	Γ_4^-
icsd_163208	As_2Fe_2Sr	69	69.523	0.00	Γ_3^-
icsd_044175	B_4Co_2Mo	71	71.535	0.00	Γ_3^-
icsd_067392	$CoCs_2Se_2$	72	72.542	2.25	Γ_2^-
icsd_067387	CoK_2S_2	72	72.542	2.72	Γ_2^-
icsd_067390	CoK_2Se_2	72	72.542	2.34	Γ_2^-
icsd_067386	$CoNa_2S_2$	72	72.542	2.45	Γ_2^-
icsd_624264	$CoNa_2Se_2$	72	72.542	1.93	Γ_2^-
icsd_067388	$CoRb_2S_2$	72	72.542	2.67	Γ_2^-
icsd_067391	$CoRb_2Se_2$	72	72.542	2.32	Γ_2^-
icsd_065455	Cs_2MnS_2	72	72.542	2.59	Γ_2^-
icsd_065458	Cs_2MnSe_2	72	72.542	2.30	Γ_2^-
icsd_065461	Cs_2MnTe_2	72	72.542	2.25	Γ_2^-
icsd_065453	K_2MnS_2	72	72.542	2.67	Γ_2^-
icsd_069870	Ca_2ClFeO_3	75	35.167	0.00	$\Gamma_3\Gamma_4$
icsd_103995	Ga_3Ti_2	83	10.44	0.00	$\Gamma_3^-\Gamma_4^-$
icsd_056880	Ca_2ClFeO_3	85	59.407	0.72	$\Gamma_3^-\Gamma_4^-$
icsd_024894	MoO_5P	85	85.62	1.88	Γ_1^-
icsd_027315	MoO_5V	85	85.62	2.23	Γ_1^-
icsd_613131	B_4Co_4La	86	13.67	0.00	$\Gamma_3^-\Gamma_4^-$
icsd_023081	$BaFe_2S_4$	87	12.60	1.35	$\Gamma_3^-\Gamma_4^-$
icsd_238713	$BaFe_2Se_4$	87	12.60	0.90	$\Gamma_3^-\Gamma_4^-$
icsd_086200	Ba_2CuHgO_5Tl	104	36.179	0.00	Γ_5
icsd_187030	AlTi	123	53.334	0.00	Γ_5^+
icsd_252344	As_4CaFe_4Rb	123	123.344	0.00	Γ_2^-
icsd_075725	$Ba_2CaCu_2HgO_6$	123	123.347	0.00	Γ_1^-
icsd_064639	$Ba_2Cu_2LaO_8Ta$	123	123.347	0.00	Γ_1^-
icsd_098113	$Ba_2Cu_3LuO_6$	123	123.347	0.00	Γ_1^-
icsd_153495	$BaCo_2LaO_6$	123	65.483	0.00	Γ_5^-
icsd_171432	$BaCo_2O_5Y$	123	123.347	0.00	Γ_1^-
icsd_083690	$BaMn_2O_5Y$	123	123.347	0.00	Γ_1^-
icsd_107586	$BiNi_9S_8Te$	123	47.251	0.00	Γ_5^-
icsd_074165	$CaCu_2O_7Sr_2Tl$	123	123.347	0.00	Γ_1^-
icsd_168904	$CaMnO_3$	123	63.466	0.00	Γ_5^+
icsd_074164	$Cu_2O_7Sr_2TlY$	123	123.347	0.00	Γ_1^-
icsd_168837	$H_2Mg_{0.5}Ti_{0.5}$	123	127.397	0.00	Γ_3^+
icsd_096951	$KO_5S_2Ti_2Y_2$	123	123.347	0.00	Γ_1^-
icsd_009967	$CoNb_4P$	124	124.353	0.00	Γ_3^-
icsd_043233	$CoNb_4Si$	124	124.353	0.00	Γ_3^-
icsd_624637	$CoPTa_4$	124	124.353	0.00	Γ_3^-
icsd_624677	$CoPZr_4$	124	124.353	0.00	Γ_3^-
icsd_086378	$FePTa_4$	124	124.353	0.00	Γ_3^-
icsd_614207	B_2FeTa_2	127	55.358	0.00	Γ_5^+
icsd_180529	$As_2Cr_2Fe_2O_6Sr_4$	129	59.407	0.00	Γ_5^-
icsd_180528	$As_2Fe_2O_6Sc_2Sr_4$	129	59.407	0.00	Γ_5^-
icsd_420654	$AsBa_2FeO_3Sc$	129	59.407	0.00	Γ_5^-
icsd_248365	AsBaFMn	129	59.407	1.22	Γ_5^-
icsd_420653	$AsCrFeO_3Sr_2$	129	59.407	0.00	Γ_5^-
icsd_237385	AsCrLaO	129	59.407	0.00	Γ_5^-
icsd_040572	AsCsMn	129	59.407	1.03	Γ_5^-
icsd_423230	AsCuMn	129	59.407	0.00	Γ_5^-
icsd_163496	AsFeLaO	129	59.407	0.00	Γ_5^-
icsd_163143	AsFeNa	129	59.407	0.73	Γ_5^-
icsd_162808	AsFFeSr	129	59.407	0.00	Γ_5^-
icsd_189940	AsFMnSr	129	59.407	1.26	Γ_5^-
icsd_041883	AsKMn	129	59.407	1.08	Γ_5^-
icsd_026459	AsLiMn	129	59.407	0.96	Γ_5^-
icsd_026461	AsMnNa	129	59.407	1.03	Γ_5^-
icsd_089596	AsMnRb	129	59.407	1.05	Γ_5^-

TABLE S45. Tabulated information on **collinear antiferromagnetic** materials, including the chemical formula, space group, magnetic space group, band gap and corresponding irreducible representations of crystallographic space group.

ICSD number	Chemical formula	SG NUM	BNS	Band Gap (eV)	Irrep
icsd_044009	AsMnV	129	59.407	0.00	Γ_5^-
icsd_426033	BaBiFMn	129	129.416	0.54	Γ_2^-
icsd_082639	$BaCoS_2$	129	67.503	0.22	Γ_5^-
icsd_248364	BaFMnSb	129	59.407	0.87	Γ_5^-
icsd_042370	BaGeMn	129	59.407	0.00	Γ_5^-
icsd_088949	$BaMn_2O_5Y$	129	129.419	0.25	Γ_1^-
icsd_015289	$BaNiS_2$	129	59.407	0.00	Γ_5^-
icsd_010454	Bi_2CaMn	129	59.407	0.00	Γ_5^-
icsd_616575	BiCsMn	129	129.416	0.19	Γ_2^-
icsd_601586	BiKMn	129	129.416	0.21	Γ_2^-
icsd_060736	BiMnNa	129	129.416	0.06	Γ_2^-
icsd_616824	BiMnRb	129	129.416	0.06	Γ_2^-
icsd_093509	$BrFeO_3Sr_2$	129	67.503	0.83	Γ_5^-
icsd_096557	Ca_2ClFeO_3	129	59.407	0.75	Γ_5^-
icsd_169992	Ca_2CuFeO_3S	129	59.407	0.63	Γ_5^-
icsd_169993	Ca_2CuFeO_3Se	129	59.407	0.72	Γ_5^-
icsd_428148	CaCoSi	129	129.416	0.00	Γ_2^-
icsd_052758	CaGeMn	129	59.407	0.00	Γ_5^-
icsd_066949	CaMnSi	129	59.407	0.00	Γ_5^-
icsd_066950	CaMnSn	129	59.407	0.00	Γ_5^-
icsd_049516	$ClFeMoO_4$	129	67.503	2.00	Γ_5^-
icsd_093508	$ClFeO_3Sr_2$	129	59.407	0.82	Γ_5^-
icsd_080798	$ClFeO_4W$	129	67.503	1.80	Γ_5^-
icsd_262357	$Co_2O_6P_2Sc_2Sr_4$	129	59.407	0.00	Γ_5^-
icsd_085860	CoGeLa	129	59.407	0.00	Γ_5^-
icsd_657919	$CoLaSb_2$	129	67.503	0.00	Γ_5^-
icsd_624027	CoLaSi	129	67.503	0.00	Γ_5^-
icsd_084962	$CrCuO_3SSr_2$	129	59.407	1.31	Γ_5^-
icsd_191256	CrN_2Nb	129	67.503	0.00	Γ_5^-
icsd_016496	CrNNb	129	59.407	0.00	Γ_5^-
icsd_162899	CrSe	129	59.407	0.00	Γ_5^-
icsd_089598	CsMnP	129	59.407	1.10	Γ_5^-
icsd_041869	CsMnSb	129	59.407	0.70	Γ_5^-
icsd_084963	$CuFeO_3SSr_2$	129	67.503	0.78	Γ_5^-
icsd_168586	$Fe_2O_6P_2Sc_2Sr_4$	129	59.407	0.00	Γ_5^-
icsd_162724	FeLaOP	129	59.407	0.00	Γ_5^-
icsd_657914	$FeLaSb_2$	129	67.503	0.00	Γ_5^-
icsd_085853	FeLaSi	129	59.407	0.00	Γ_5^-
icsd_042327	FeLiP	129	59.407	0.00	Γ_5^-
icsd_042977	FeS	129	59.407	1.33	Γ_5^-
icsd_026889	FeSe	129	59.407	1.28	Γ_5^-
icsd_633643	FeSiY	129	59.407	0.00	Γ_5^-
icsd_044753	FeTe	129	59.407	0.45	Γ_5^-
icsd_088460	$FFeO_3Sr_2$	129	67.503	0.70	Γ_5^-
icsd_189939	FMnPSr	129	59.407	1.39	Γ_5^-
icsd_189941	FMnSbSr	129	59.407	0.86	Γ_5^-
icsd_634253	GaGeMn	129	59.407	0.00	Γ_5^-
icsd_636594	GeHfV	129	59.407	0.00	Γ_5^-
icsd_080007	GeLaMn	129	59.407	0.00	Γ_5^-
icsd_088209	GeLuTi	129	59.407	0.00	Γ_5^-
icsd_066948	GeMgMn	129	59.407	0.00	Γ_5^-
icsd_053707	GeMnSr	129	59.407	0.00	Γ_5^-
icsd_638931	HfSiV	129	59.407	0.00	Γ_5^-
icsd_041882	KMnP	129	59.407	1.46	Γ_5^-
icsd_089590	KMnSb	129	59.407	1.04	Γ_5^-
icsd_419355	LaMnOSb	129	59.407	0.76	Γ_5^-
icsd_075046	LaMnSi	129	59.407	0.00	Γ_5^-
icsd_026458	LiMnP	129	59.407	1.05	Γ_5^-
icsd_642150	LiMnSb	129	59.407	0.37	Γ_5^-
icsd_026460	MnNaP	129	59.407	1.19	Γ_5^-
icsd_026462	MnNaSb	129	59.407	0.71	Γ_5^-
icsd_089594	MnPRb	129	59.407	1.36	Γ_5^-
icsd_041868	MnRbSb	129	59.407	0.90	Γ_5^-
icsd_162900	MnSe	129	59.407	0.68	Γ_5^-
icsd_076235	MnSiY	129	59.407	0.00	Γ_5^-

TABLE S46. Tabulated information on **collinear antiferromagnetic** materials, including the chemical formula, space group, magnetic space group, band gap and corresponding irreducible representations of crystallographic space group.

ICSD number	Chemical formula	SG NUM	BNS	Band Gap (eV)	Irrep
icsd_066951	MnSnSr	129	59.407	0.00	Γ_5^-
icsd_162897	SeTi	129	59.407	0.00	Γ_5^-
icsd_162898	SeV	129	59.407	0.00	Γ_5^-
icsd_042337	SiVZr	129	59.407	0.00	Γ_5^-
icsd_412062	Co_4In_{12}	136	58.398	0.00	Γ_5^+
icsd_020314	Cr_2O_6W	136	136.502	0.99	Γ_4^-
icsd_015306	CrO_6Ta_2	136	58.398	0.00	Γ_5^+
icsd_024795	Fe_2O_6Te	136	136.503	1.74	Γ_1^-
icsd_186045	Fe_4Ge_2Lu	136	58.395	0.00	Γ_5^-
icsd_186048	Fe_4Si_2Y	136	58.395	0.00	Γ_5^-
icsd_103447	$FeGa_3$	136	58.395	0.00	Γ_5^-
icsd_002575	O_6V_2W	136	136.502	1.28	Γ_4^-
icsd_074985	B_4Mn_4	138	67.503	0.00	Γ_5^-
icsd_609848	As_2BaCo_2	139	71.535	0.00	Γ_5^-
icsd_166018	As_2BaFe_2	139	69.523	0.00	Γ_5^-
icsd_609899	As_2CaCo_2	139	71.535	0.00	Γ_5^-
icsd_610073	As_2Co_2La	139	69.523	0.00	Γ_5^-
icsd_610122	As_2Co_2Sr	139	71.535	0.00	Γ_5^-
icsd_074877	As_2CsFe_2	139	139.536	0.00	Γ_2^-
icsd_163209	As_2Fe_2Sr	139	71.535	0.00	Γ_5^-
icsd_023653	B_2Co_2Y	139	71.535	0.00	Γ_5^-
icsd_252590	$BaBi_2Mn_2$	139	71.535	0.00	Γ_5^-
icsd_010468	$BaFe_2P_2$	139	69.523	0.00	Γ_5^-
icsd_000405	$BaMn_2Sn_2$	139	139.536	0.00	Γ_2^-
icsd_000406	$CaCo_2Ge_2$	139	71.535	0.00	Γ_5^-
icsd_010462	$CaCo_2P_2$	139	139.536	0.00	Γ_2^-
icsd_081748	Co_2Ge_2Y	139	69.523	0.00	Γ_5^-
icsd_100438	Co_2S_2Tl	139	139.536	0.00	Γ_2^-
icsd_624957	Co_2ScSi_2	139	71.535	0.00	Γ_5^-
icsd_626238	Cr_2LuSi_2	139	139.536	0.00	Γ_2^-
icsd_633666	Fe_2Si_2Zr	139	139.536	0.00	Γ_2^-
icsd_641273	KNi_2S_2	139	139.536	0.00	Γ_2^-
icsd_424686	KNi_2Se_2	139	139.536	0.00	Γ_2^-
icsd_646396	Ni_2S_2Tl	139	139.536	0.00	Γ_2^-
icsd_646550	Ni_2Se_2Tl	139	139.536	0.00	Γ_2^-
icsd_086811	$CrSb_2$	140	140.543	0.00	Γ_3^-
icsd_042520	Sb_2Ti	140	140.543	0.00	Γ_3^-
icsd_425309	BFe	141	70.529	0.00	Γ_5^-
icsd_043437	$FeLiO_2$	141	141.556	1.22	Γ_2^-
icsd_164158	LiO_2Ti	141	141.556	0.66	Γ_2^-
icsd_250709	$BaCo_2O_8P_2$	147	147.15	2.76	Γ_1^-
icsd_417824	$C_6FeMn_2N_6$	147	147.15	3.77	Γ_1^-
icsd_417825	$C_6Mn_2N_6Os$	147	147.15	3.30	Γ_1^-
icsd_417823	$C_6Mn_2N_6Ru$	147	147.15	3.65	Γ_1^-
icsd_164936	$CrLaO_6Te$	147	15.87	0.88	$\Gamma_2^-\Gamma_3^-$
icsd_027014	$As_2BaNi_2O_8$	148	2.6	2.85	$\Gamma_2^-\Gamma_3^-$
icsd_063353	$AsNaNiO_4$	148	2.6	3.34	$\Gamma_2^-\Gamma_3^-$
icsd_059343	$BaCo_2O_8P_2$	148	148.19	3.56	Γ_1^-
icsd_280167	$BaNi_2O_8P_2$	148	2.6	3.84	$\Gamma_2^-\Gamma_3^-$
icsd_041540	$Br_{12}Zr_6$	148	148.19	0.24	Γ_1^-
icsd_408324	$Ca_2Li_6Mn_2N_6$	148	148.19	1.53	Γ_1^-
icsd_041539	$Cl_{12}Zr_6$	148	148.19	0.17	Γ_1^-
icsd_027500	Cl_3Fe	148	148.19	2.11	Γ_1^-
icsd_038236	Cl_3Ti	148	2.6	2.24	$\Gamma_2^-\Gamma_3^-$
icsd_031854	$CoMnO_3$	148	148.19	0.68	Γ_1^-
icsd_087943	F_3Ni	148	2.4	1.46	$\Gamma_2^+\Gamma_3^+$
icsd_056890	$Fe_2P_2Se_6$	148	2.6	1.98	$\Gamma_2^-\Gamma_3^-$
icsd_024790	FeO_3Ti	148	2.6	1.89	$\Gamma_2^-\Gamma_3^-$
icsd_054141	$FePSe_3$	148	2.6	1.50	$\Gamma_2^-\Gamma_3^-$
icsd_069591	$GeMnO_3$	148	2.6	2.36	$\Gamma_2^-\Gamma_3^-$
icsd_281462	$HCa_6Cr_2N_6$	148	148.19	0.00	Γ_1^-
icsd_412874	$Li_6Mn_2N_6Sr_2$	148	148.19	1.43	Γ_1^-
icsd_643237	$Mn_2P_2Se_6$	148	2.6	1.67	$\Gamma_2^-\Gamma_3^-$
icsd_029203	MnO_3Sn	148	2.6	1.30	$\Gamma_2^-\Gamma_3^-$
icsd_044407	MnO_3Ti	148	2.6	2.91	$\Gamma_2^-\Gamma_3^-$

TABLE S47. Tabulated information on **collinear antiferromagnetic** materials, including the chemical formula, space group, magnetic space group, band gap and corresponding irreducible representations of crystallographic space group.

ICSD number	Chemical formula	SG NUM	BNS	Band Gap (eV)	Irrep
icsd_054140	$MnPSe_3$	148	2.6	1.66	$\Gamma_2^-\Gamma_3^-$
icsd_015988	NiO_3Ti	148	2.6	2.82	$\Gamma_2^-\Gamma_3^-$
icsd_017009	OTi_6	159	163.82	0.00	Γ_2
icsd_029035	Cl_3Ti	162	12.60	2.16	Γ_3^-
icsd_248351	O_6Ru_2Sr	162	162.75	1.10	Γ_2^-
icsd_032730	$CaCoF_6Li$	163	15.87	2.86	Γ_3^-
icsd_032732	CaF_6LiNi	163	15.88	2.34	Γ_3^-
icsd_032731	$CdCoF_6Li$	163	15.87	2.52	Γ_3^-
icsd_039428	Cl_3Ti	163	15.87	2.23	Γ_3^-
icsd_039817	Cl_6FeHf	163	163.81	3.04	Γ_2^-
icsd_039666	Cl_6FeZr	163	15.87	3.24	Γ_3^-
icsd_183024	Cl_6MoNa_3	163	15.87	2.93	Γ_3^-
icsd_032733	$F_6LiNiSr$	163	15.88	2.34	Γ_3^-
icsd_020042	OTi_6	163	162.76	0.00	Γ_1^-
icsd_041793	As_2Mn_2Sr	164	12.60	0.51	Γ_3^-
icsd_039512	As_2Mn_2Zn	164	12.60	0.00	Γ_3^-
icsd_429102	$As_5La_4Mn_2$	164	12.61	0.00	Γ_3^-
icsd_152482	$Ba_3CaO_9Ru_2$	164	164.88	1.33	Γ_1^-
icsd_041791	Bi_2CaMn_2	164	12.60	0.16	Γ_3^-
icsd_041789	$CaMn_2Sb_2$	164	12.60	0.39	Γ_3^-
icsd_022074	$Cl_9Cs_3Fe_2$	164	164.88	0.81	Γ_1^-
icsd_631804	$Fe_2Ga_2S_5$	164	12.60	0.72	Γ_3^-
icsd_159909	$Fe_2K_3NaO_8$	164	12.60	1.77	Γ_3^-
icsd_200009	Fe_2NaO_3	164	164.88	0.00	Γ_1^-
icsd_634664	$Ga_2Mn_2S_5$	164	164.88	0.47	Γ_1^-
icsd_416040	$K_3NaO_8Ru_2$	164	12.60	1.26	Γ_3^-
icsd_073874	Li_2NiO_2	164	165.96	3.46	Γ_2^+
icsd_041790	Mn_2Sb_2Sr	164	12.61	0.34	Γ_3^-
icsd_416038	$NaO_8Rb_3Ru_2$	164	12.60	1.26	Γ_3^-
icsd_023574	OTi_2	164	164.88	0.00	Γ_1^-
icsd_151457	AlO_4V_2	166	12.58	0.00	Γ_3^+
icsd_025005	Ba_2NiO_6Te	166	166.100	2.85	Γ_1^-
icsd_280045	$Ba_3Mn_2O_8$	166	12.60	1.81	Γ_3^-
icsd_085055	$Cr_2O_8Sr_3$	166	166.100	0.61	Γ_1^-
icsd_078928	$Cs_4F_{12}Fe_2KLi$	166	12.60	3.96	Γ_3^-
icsd_157323	Fe_2InO_4	166	166.100	0.00	Γ_1^-
icsd_041381	Fe_6Ge_4Li	166	166.100	0.00	Γ_1^-
icsd_029011	FeO_2Tl	166	166.100	1.11	Γ_1^-
icsd_099369	$CoLaO_3$	167	15.85	1.51	Γ_3^+
icsd_025781	Cr_2O_3	167	167.106	2.47	Γ_1^-
icsd_026629	F_3Mo	167	15.85	2.88	Γ_3^+
icsd_001473	O_3V_2	167	15.88	1.04	Γ_3^-
icsd_036502	Ba_3FeN_3	176	11.53	0.00	$\Gamma_3^-\Gamma_5^-$
icsd_095740	$CBaF_2MnO_3$	176	176.145	4.29	Γ_2^-
icsd_057518	Al_9BaFe_2	191	191.236	0.00	Γ_3^-
icsd_623434	Co_6Ge_6Hf	191	191.241	0.00	Γ_1^-
icsd_041459	Co_6Ge_6Li	191	191.241	0.00	Γ_1^-
icsd_623474	Co_6Ge_6Lu	191	191.241	0.00	Γ_1^-
icsd_415256	Co_6Ge_6Mg	191	191.241	0.00	Γ_1^-
icsd_623581	Co_6Ge_6Sc	191	191.241	0.00	Γ_1^-
icsd_041460	Co_6Ge_6Zr	191	191.241	0.00	Γ_1^-
icsd_191489	BSi_3V_5	193	193.257	0.00	Γ_4^-
icsd_648274	P_3V_5	193	63.461	0.00	Γ_5^-
icsd_172878	$Ag_3Ni_2O_4$	194	63.461	0.00	Γ_5^-
icsd_261608	$AgCoO_2$	194	63.461	0.00	Γ_5^-
icsd_181348	AlN_3V_4	194	63.461	0.00	Γ_5^-
icsd_058188	$AlTi_3$	194	63.461	0.00	Γ_5^-
icsd_016773	$AsTi$	194	63.461	0.00	Γ_5^-
icsd_670859	B_4Fe	194	194.266	0.00	Γ_3^-
icsd_016361	$Ba_2Bi_2Mn_2O$	194	194.271	0.06	Γ_1^-
icsd_016360	$Ba_2Mn_2OSb_2$	194	194.271	0.34	Γ_1^-
icsd_058697	Be_2Cr	194	63.460	0.53	Γ_6^-
icsd_058714	Be_2Mn	194	63.461	0.00	Γ_5^-
icsd_058752	Be_2V	194	63.461	0.00	Γ_5^-
icsd_080373	C_2CrSc	194	194.266	0.00	Γ_3^-

TABLE S48. Tabulated information on **collinear antiferromagnetic** materials, including the chemical formula, space group, magnetic space group, band gap and corresponding irreducible representations of crystallographic space group.

ICSD number	Chemical formula	SG NUM	BNS	Band Gap (eV)	Irrep
icsd_042918	$CAlCr_2$	194	63.465	0.00	Γ_5^-
icsd_043874	$CAsV_2$	194	63.461	0.00	Γ_5^-
icsd_076802	CCr_2Ge	194	63.461	0.00	Γ_5^-
icsd_183361	CCr_2Si	194	63.465	0.00	Γ_5^-
icsd_162103	CFe_2	194	63.466	0.00	Γ_5^+
icsd_042919	$CGeV_2$	194	194.271	0.00	Γ_1^-
icsd_163505	$CInV_2$	194	194.271	0.00	Γ_1^-
icsd_300249	Cl_3CsFe	194	63.462	3.42	Γ_5^+
icsd_670893	CMo	194	63.461	0.00	Γ_5^-
icsd_625123	$Co_{1.5}Si_{0.5}W$	194	63.465	0.00	Γ_5^-
icsd_052972	Co_3GeMn_2	194	194.266	0.00	Γ_3^-
icsd_181100	$CPTa_2$	194	63.461	0.00	Γ_5^-
icsd_029284	CPV_2	194	63.461	0.00	Γ_5^-
icsd_049666	CrS	194	194.268	0.00	Γ_4^+
icsd_633437	$Fe_{1.5}ScSi_{0.5}$	194	194.266	0.00	Γ_3^-
icsd_049912	$Fe_2Ga_2S_5$	194	63.460	0.74	Γ_6^-
icsd_071010	$FeInO_3$	194	194.266	0.77	Γ_3^-
icsd_103991	$GaTi_3$	194	63.461	0.00	Γ_5^-
icsd_636809	$GeLaLi_2$	194	63.461	0.00	Γ_5^-
icsd_052020	$GeMn_2$	194	63.464	0.00	Γ_6^+
icsd_640656	$InTi_3$	194	194.266	0.00	Γ_3^-
icsd_104976	Mn_2Sn	194	63.463	0.00	Γ_6^+
icsd_157935	MnO_3Sr	194	63.459	1.82	Γ_6^-
icsd_290431	N_2Ta	194	63.461	0.00	Γ_5^-
icsd_106086	$SnTi_2$	194	63.463	0.00	Γ_6^+
icsd_150657	$SnTi_3$	194	63.465	0.00	Γ_5^-
icsd_044764	MnS	219	167.108	0.00	Γ_4
icsd_058200	AlV_3	223	167.105	0.00	Γ_4^-
icsd_044084	AsV_3	223	167.105	0.00	Γ_4^-
icsd_020212	GeV_3	223	167.105	0.00	Γ_4^-
icsd_105639	PbV_3	223	167.105	0.00	Γ_4^-
icsd_106097	SnV_3	223	167.105	0.00	Γ_4^-
icsd_057648	$AlCo_2Zr$	225	166.100	0.00	Γ_5^-
icsd_057808	$AlFe_2Ni$	225	166.100	0.00	Γ_5^-
icsd_102433	Co_2GaHf	225	71.535	0.00	Γ_5^-
icsd_169731	Co_2GaNi	225	166.100	0.00	Γ_5^-
icsd_025324	Co_2GeLi	225	166.100	0.00	Γ_5^-
icsd_052994	Co_2GeZn	225	166.100	0.00	Γ_5^-
icsd_102646	Co_2ScSn	225	71.535	0.00	Γ_5^-
icsd_103460	Fe_2GaNi	225	139.536	0.00	Γ_5^-
icsd_186057	Fe_2GeTi	225	71.535	0.04	Γ_5^-

F. Noncollinear Antiferromagnetic Materials

The relevant information for noncollinear antiferromagnetic materials is summarized in Table S49-S50, including their chemical formula, space group, magnetic space group, band gap and corresponding irreducible representations of crystallographic space group.

TABLE S49. Tabulated information on **noncollinear antiferromagnetic** materials, including the chemical formula, space group, magnetic space group, band gap and corresponding irreducible representations of crystallographic space group.

ICSD number	Chemical formula	SG NUM	BNS	Band Gap (eV)	Irrep
icsd_000453	$Ni_3S_2Sn_2$	12	12.58	0.00	Γ_1^+
icsd_186046	Fe_4Ge_2Lu	58	58.396	0.00	Γ_2^-
icsd_670828	$CFeMn_2$	62	62.441	0.00	Γ_1^+
icsd_185418	MnO_3V	62	62.441	0.78	Γ_1^+
icsd_057009	C_2Cr_3	63	63.465	0.00	Γ_1^-
icsd_609880	$CAsCr_3$	63	63.465	0.00	Γ_1^-
icsd_291338	CCr_3P	63	63.459	0.00	Γ_3^-
icsd_291339	Cr_3NP	63	63.464	0.00	Γ_4^+
icsd_180767	Ni_3S_2	63	63.459	0.00	Γ_3^-
icsd_644620	NPV_3	63	63.465	0.00	Γ_1^-
icsd_055075	Se_4Ti_5	87	87.79	0.01	Γ_2^-
icsd_015451	Te_4Ti_5	87	87.78	0.05	Γ_1^-
icsd_102500	$CoIn_3$	118	34.158	0.00	Γ_5
icsd_042335	$AsCr_2$	129	67.503	0.00	Γ_5^-
icsd_024794	Cr_2O_6Te	136	58.395	1.74	Γ_5^-
icsd_078778	CrF_4	136	136.502	1.19	Γ_4^-
icsd_613152	B_4Co_4Lu	137	137.510	0.00	Γ_4^+
icsd_613410	B_4Co_4Y	137	137.510	0.00	Γ_4^+
icsd_025760	$AsCr_3N$	140	140.543	0.00	Γ_3^-
icsd_182435	Mn_3O_6Te	148	2.6	1.68	$\Gamma_2^-\Gamma_3^-$
icsd_016316	Mo_3Se_4	148	1.1	0.00	Γ_1^-
icsd_020389	Fe_3N	149	182.181	0.00	Γ_1
icsd_025813	$BaCoO_2$	152	5.13	2.11	Γ_3
icsd_004266	FeO_4P	152	152.35	2.69	Γ_2
icsd_010424	Ni_3S_2	155	5.15	0.00	Γ_3
icsd_401027	$Cl_8Na_2Ti_3$	160	8.32	1.85	Γ_3
icsd_036207	Fe_3O_7P	160	160.67	2.31	Γ_2
icsd_029312	NiS	160	160.65	0.00	Γ_1
icsd_042596	NiSe	160	8.32	0.00	Γ_3
icsd_001846	$Cl_8Mn_3Na_2$	166	166.101	4.28	Γ_2^+
icsd_401026	$Cl_8Na_2Ti_3$	166	166.97	2.53	Γ_1^+
icsd_291388	$Cs_2Cu_3F_{12}Sn$	166	12.62	3.55	Γ_3^+
icsd_425834	$H_6Cl_2Cu_3O_6Zn$	166	12.62	2.25	Γ_3^+
icsd_024176	$Ni_3Pb_2S_2$	166	166.97	0.00	Γ_1^+
icsd_100217	$Ni_3S_2Sn_2$	166	12.58	0.00	Γ_3^+
icsd_094318	$BLiMnO_3$	174	174.135	2.94	Γ_2
icsd_072920	S_4V_3	176	11.53	0.00	$\Gamma_3^-\Gamma_5^-$
icsd_638088	Ge_2V	180	180.169	0.00	Γ_4
icsd_168997	FeO_4P	181	21.41	3.13	Γ_6
icsd_069692	Co_6LiP_4	187	187.211	0.00	Γ_4
icsd_094412	Co_6MgP_4	187	187.211	0.00	Γ_4
icsd_251064	$Ag_2S_6TeV_3$	189	189.224	0.00	Γ_2
icsd_610509	AsFeNi	189	189.223	0.00	Γ_3
icsd_610530	AsFeTi	189	189.223	0.00	Γ_3
icsd_610532	AsFeV	189	38.191	0.00	Γ_6
icsd_614205	BFeTa	189	38.191	0.00	Γ_6
icsd_042735	CoSiTi	189	189.223	0.00	Γ_3
icsd_002278	$CrCsF_4$	189	189.224	2.12	Γ_2
icsd_042060	CrNbSi	189	38.191	0.00	Γ_6
icsd_042402	Fe_2P	189	38.191	0.00	Γ_6
icsd_086364	FeGeSc	189	38.191	0.00	Γ_6
icsd_632938	FeNiP	189	189.223	0.00	Γ_3
icsd_290889	FePTi	189	189.224	0.00	Γ_2
icsd_099080	$Ga_2Lu_3Mn_3Si$	189	189.223	0.00	Γ_3
icsd_409925	GePdTi	189	38.189	0.00	Γ_6
icsd_410967	$In_3Rh_2Ti_3$	189	189.223	0.00	Γ_3
icsd_086369	MnScSi	189	189.223	0.00	Γ_3
icsd_643653	MnSiTa	189	189.224	0.00	Γ_2
icsd_023550	B_2Co_3Hf	191	191.238	0.00	Γ_4^+
icsd_044171	B_2Co_3Lu	191	65.486	0.00	Γ_6^+
icsd_044179	B_2Co_3Sc	191	191.238	0.00	Γ_4^+
icsd_023655	B_2Co_3Y	191	191.238	0.00	Γ_4^+
icsd_044191	B_2Co_3Zr	191	191.238	0.00	Γ_4^+
icsd_089437	Ge_6Mn_6Sc	191	191.237	0.00	Γ_4^-
icsd_240144	Mn_6Sn_6Y	191	65.486	0.00	Γ_6^+

TABLE S50. Tabulated information on **noncollinear antiferromagnetic** materials, including the chemical formula, space group, magnetic space group, band gap and corresponding irreducible representations of crystallographic space group.

ICSD number	Chemical formula	SG NUM	BNS	Band Gap (eV)	Irrep
icsd_182148	Sn_6V_6Y	191	65.486	0.00	Γ_6^+
icsd_635612	Ga_3V_5	193	193.259	0.00	Γ_3^+
icsd_044504	Ge_3V_5	193	193.259	0.00	Γ_3^+
icsd_191487	Si_3V_5	193	193.259	0.00	Γ_3^+
icsd_109292	Sn_3Ti_5	193	193.255	0.00	Γ_2^-
icsd_187992	$AlCo_3$	194	194.269	0.00	Γ_3^+
icsd_603351	$GaMn_3$	194	63.463	0.00	Γ_6^+
icsd_603343	$GeMn_3$	194	63.464	0.00	Γ_6^+
icsd_104978	Mn_3Sn	194	63.464	0.00	Γ_6^+
icsd_652343	$SiTa_2V_3$	194	194.271	0.00	Γ_1^-
icsd_106098	SnV_3	194	194.268	0.00	Γ_4^+
icsd_093901	AsNiSe	198	198.9	0.00	Γ_1
icsd_624862	CoSSb	198	19.25	0.24	$\Gamma_2\Gamma_3$
icsd_100568	F_2Pd	198	198.9	1.54	Γ_1
icsd_187195	GeMn	198	146.10	0.00	Γ_4
icsd_038843	NiSSb	198	198.9	0.00	Γ_1
icsd_041209	F_2Pd	205	205.33	1.54	Γ_1^+
icsd_633869	$FeTe_2$	205	61.433	0.00	$\Gamma_2^+\Gamma_3^+$
icsd_024021	$MnTe_2$	205	205.33	0.49	Γ_1^+
icsd_040328	NiS_2	205	205.33	0.54	Γ_1^+
icsd_040330	$NiSe_2$	205	61.436	0.19	Γ_4^+
icsd_608469	$Al_{0.6}Mn_{0.4}$	213	92.115	0.00	Γ_5
icsd_044729	CFe_4	215	111.255	0.00	Γ_5
icsd_052642	$AlNTi_3$	221	8.34	0.00	Γ_4^+
icsd_053141	Cr_3NPd	221	166.97	0.00	Γ_5^+
icsd_053142	Cr_3NPt	221	166.101	0.00	Γ_4^+
icsd_168836	$H_2Mg_{0.25}Ti_{0.75}$	221	166.97	0.00	Γ_5^+
icsd_193569	$MgNi_3$	221	5.13	0.00	Γ_5^+
icsd_102767	Cr_3Ga	223	167.105	0.00	Γ_4^-
icsd_053127	Cr_3Ge	223	167.106	0.00	Γ_5^-
icsd_015904	Cr_3O	223	2.6	0.00	Γ_5^-
icsd_016835	Cr_3Si	223	167.106	0.00	Γ_5^-
icsd_104020	GaV_3	223	167.106	0.00	Γ_5^-
icsd_611953	H_3AuTi_3	223	167.105	0.00	Γ_4^-
icsd_052330	SbV_3	223	223.106	0.00	Γ_2^-
icsd_022412	SiV_3	223	167.106	0.00	Γ_5^-

G. Altermagnetic Materials

The relevant information for altermagnetic materials is summarized in Table S51-S57, including their chemical formula, space group, magnetic space group, band gap and corresponding irreducible representations of crystallographic space group.

TABLE S51. Tabulated information on **altermagnetic** materials, including the chemical formula, space group, magnetic space group, band gap and corresponding irreducible representations of crystallographic space group.

ICSD number	Chemical formula	SG NUM	BNS	Band Gap (eV)	Irrep
icsd_084868	$CaCuO_2$	4	4.7	1.25	Γ_1
icsd_004327	CuI_2O_6	4	4.9	2.16	Γ_2
icsd_020157	F_6FeNa_3	4	4.7	3.94	Γ_1
icsd_008010	FeI_4Rb_2	4	4.9	2.57	Γ_2
icsd_237487	$FeLaNaO_6W$	4	4.7	1.48	Γ_1
icsd_238786	$K_2La_2Mn_2O_{12}W_2$	4	4.7	2.16	Γ_1
icsd_238788	$K_2Mn_2O_{12}W_2Y_2$	4	4.9	2.39	Γ_2
icsd_238789	$La_2Mn_2Na_2O_{12}W_2$	4	4.7	1.94	Γ_1
icsd_238785	$La_2Mn_2O_{12}Rb_2W_2$	4	4.7	2.16	Γ_1
icsd_159097	$LaMnNaO_6W$	4	4.7	2.23	Γ_1
icsd_238791	$Mn_2Na_2O_{12}W_2Y_2$	4	4.7	2.33	Γ_1
icsd_238793	$Mn_2O_{12}Rb_2W_2Y_2$	4	4.9	2.42	Γ_2
icsd_084830	$H_2BaCo_2O_9P_2$	5	5.13	3.78	Γ_1
icsd_425760	Ag_2FeS_4Si	7	7.26	2.04	Γ_2
icsd_039528	Br_7FeSe	7	7.24	1.91	Γ_1
icsd_200680	$CoGeNa_2O_4$	7	7.24	2.46	Γ_1
icsd_238234	$FeGeLi_2S_4$	7	7.26	2.23	Γ_2
icsd_238236	$FeLi_2S_4Sn$	7	7.26	2.30	Γ_2
icsd_281242	I_6K_2Re	7	7.24	0.67	Γ_1
icsd_429816	Li_2MnS_4Sn	7	7.24	2.25	Γ_1
icsd_192515	$BiFeO_3$	9	9.39	2.09	Γ_2
icsd_010501	$CoNa_4O_3$	9	9.39	1.89	Γ_2
icsd_069757	CuO	9	9.39	1.07	Γ_2
icsd_001410	$FeNa_4O_3$	9	9.39	1.56	Γ_2
icsd_060759	CuF_2O_3W	11	11.50	2.68	Γ_1^+
icsd_252429	H_3ClCuO_3Zn	11	11.50	2.55	Γ_1^+
icsd_036582	$HCuO_5SeTl$	11	11.50	2.26	Γ_1^+
icsd_036581	$HCuO_5STl$	11	11.50	2.24	Γ_1^+
icsd_020453	AgF_2	14	14.79	0.00	Γ_2^+
icsd_425149	AgF_4Na_2	14	14.75	0.98	Γ_1^+
icsd_425100	B_4Mn	14	14.75	0.00	Γ_1^+
icsd_100793	Ba_2LaO_6Ru	14	14.79	1.34	Γ_2^+
icsd_190774	C_2NiO_4	14	14.75	1.82	Γ_1^+
icsd_153001	Ca_2CoO_6Te	14	14.75	2.71	Γ_1^+
icsd_098732	Ca_2CoO_6W	14	14.75	2.50	Γ_1^+
icsd_083473	Ca_2FeO_6Sb	14	14.75	2.04	Γ_1^+
icsd_051615	Ca_2MnO_6W	14	14.75	1.94	Γ_1^+
icsd_098733	Ca_2NiO_6W	14	14.75	2.84	Γ_1^+
icsd_079451	$CaIrO_6Sr_2$	14	14.75	0.22	Γ_1^+
icsd_250364	Cl_4V	14	14.75	1.43	Γ_1^+
icsd_411050	Cl_6Na_3Ti	14	14.75	2.71	Γ_1^+
icsd_202918	CoF_4Li	14	14.75	2.77	Γ_1^+
icsd_169193	CoO_6Pb_2Te	14	14.75	2.33	Γ_1^+
icsd_153002	CoO_6Sr_2Te	14	14.79	1.74	Γ_2^+
icsd_188476	$Cr_{0.5}Mn_{0.5}O_3Y$	14	14.75	0.59	Γ_1^+
icsd_031827	CrF_2	14	14.75	2.13	Γ_1^+
icsd_006024	CuF_2	14	14.75	3.22	Γ_1^+
icsd_034602	CuF_4Na_2	14	14.75	3.85	Γ_1^+
icsd_065785	F_4V	14	14.79	2.81	Γ_2^+
icsd_172591	FeO_6Sr_2Ta	14	14.75	1.88	Γ_1^+
icsd_024161	$FeSSb$	14	14.75	0.00	Γ_1^+
icsd_098698	$HCuFO$	14	14.75	3.01	Γ_1^+
icsd_065510	I_6K_2Tc	14	14.75	1.09	Γ_1^+
icsd_097487	La_2LiO_6Ru	14	14.75	1.33	Γ_1^+
icsd_170175	La_2NaO_6Os	14	14.75	1.20	Γ_1^+
icsd_160372	La_2NaO_6Ru	14	14.75	1.52	Γ_1^+
icsd_073900	LaO_3V	14	14.75	1.78	Γ_1^+
icsd_202866	LuO_6RuSr_2	14	14.75	1.29	Γ_1^+
icsd_097744	$MnMoO_6Sr_2$	14	14.75	0.91	Γ_1^+
icsd_097745	MnO_6Sr_2W	14	14.75	1.62	Γ_1^+
icsd_193723	MnS_2	14	14.75	0.00	Γ_1^+
icsd_095578	O_3VY	14	14.75	1.93	Γ_1^+
icsd_238311	O_6OsSr_2Y	14	14.79	0.81	Γ_2^+
icsd_049500	O_6RuSr_2Y	14	14.75	1.24	Γ_1^+
icsd_099370	$CoLaO_3$	15	15.89	1.55	Γ_2^+

TABLE S52. Tabulated information on **altermagnetic** materials, including the chemical formula, space group, magnetic space group, band gap and corresponding irreducible representations of crystallographic space group.

ICSD number	Chemical formula	SG NUM	BNS	Band Gap (eV)	Irrep
icsd_016723	CrS	15	15.85	0.56	Γ_1^+
icsd_016025	CuO	15	15.89	1.07	Γ_2^+
icsd_093795	$CoMoO_6Te$	18	18.19	2.50	Γ_4
icsd_163978	$MnMoO_6Te$	18	18.19	2.61	Γ_4
icsd_187196	GeMn	19	19.27	0.00	Γ_3
icsd_075401	$CCuFKO_3$	26	26.70	1.38	Γ_2
icsd_031189	AsCoS	29	29.99	0.82	Γ_1
icsd_023425	$CoGeNa_2O_4$	31	31.123	0.92	Γ_1
icsd_627355	Cu_2FeS_4Si	31	31.123	1.49	Γ_1
icsd_042490	Cu_2GeMnS_4	31	31.127	0.92	Γ_2
icsd_193986	Cu_2MnS_4Si	31	31.125	2.26	Γ_4
icsd_628396	Cu_2MnSe_4Si	31	31.127	1.35	Γ_2
icsd_161306	$FeLi_2O_4Si$	31	31.123	2.48	Γ_1
icsd_071177	H_2KMnO_5P	31	31.125	3.73	Γ_4
icsd_087325	$HFeO_2$	31	31.127	1.97	Γ_2
icsd_161305	Li_2MnO_4Si	31	31.125	3.34	Γ_4
icsd_670672	Li_2MnS_4Sn	31	31.127	1.80	Γ_2
icsd_015065	AsCo	33	33.148	0.00	Γ_2
icsd_015009	AsFe	33	33.144	0.00	Γ_1
icsd_042445	AsV	33	33.148	0.00	Γ_2
icsd_027117	$FeNaO_2$	33	33.148	2.99	Γ_2
icsd_023822	FeO_3Y	33	33.148	2.62	Γ_2
icsd_015057	FeP	33	33.144	0.00	Γ_1
icsd_023528	$GeMnN_2$	33	33.146	0.89	Γ_4
icsd_157925	HLaNiSn	33	62.444	0.00	Γ_1
icsd_023527	MnN_2Si	33	33.146	2.21	Γ_4
icsd_015003	$FeSb_2$	34	34.156	0.00	Γ_1
icsd_001544	$HFeO_2$	36	36.174	0.00	Γ_4
icsd_430557	Fe_2O_3	41	41.211	0.44	Γ_1
icsd_025754	$CuGeO_3$	51	51.294	2.27	Γ_2^+
icsd_089669	CuO_3Si	51	51.294	2.57	Γ_2^+
icsd_670125	CuO_2Pt	53	53.326	0.59	Γ_2^+
icsd_009136	Cl_4MnNa_2	55	55.358	4.18	Γ_4^+
icsd_400264	Cl_4Na_2Ti	55	55.353	2.55	Γ_1^+
icsd_022046	$GeMn_2O_4$	55	55.358	1.91	Γ_4^+
icsd_041724	As_2Fe	58	58.393	0.00	Γ_1^+
icsd_196424	B_4Fe	58	58.398	0.00	Γ_4^+
icsd_194807	B_4Mn	58	58.393	0.00	Γ_1^+
icsd_419222	$C_2H_2FeN_4$	58	58.393	3.07	Γ_1^+
icsd_034307	F_2Ni	58	58.398	4.43	Γ_4^+
icsd_015027	FeP_2	58	58.398	0.00	Γ_3^+
icsd_041727	$FeSb_2$	58	58.393	0.00	Γ_1^+
icsd_025680	$FeSe_2$	58	58.393	0.00	Γ_1^+
icsd_041123	$H_4O_4V_2$	58	58.398	0.00	Γ_3^+
icsd_643441	MnS_2	58	58.398	0.00	Γ_4^+
icsd_169570	NiS_2	58	58.398	0.00	Γ_3^+
icsd_005071	$NiSe_2$	58	58.393	0.00	Γ_1^+
icsd_084619	O_2Ru	58	58.393	0.00	Γ_1^+
icsd_082689	CaO_5V_2	59	59.410	2.13	Γ_3^+
icsd_015522	Cl_3CuRb	60	60.422	1.40	Γ_2^+
icsd_023382	$CrCsI_3$	60	60.417	0.95	Γ_1^+
icsd_020365	F_2Mn	60	60.422	3.48	Γ_2^+
icsd_152811	Fe_2N	60	60.417	0.00	Γ_1^+
icsd_096077	Fe_2O_3	60	60.424	1.47	Γ_4^+
icsd_006277	AgF_2	61	61.436	0.43	Γ_4^+
icsd_291504	MnS_2	61	61.436	0.99	Γ_3^+
icsd_610089	AsCoNb	62	62.441	0.00	Γ_1^+
icsd_041893	B_2CoNb	62	62.441	0.00	Γ_1^+
icsd_613324	B_2CoTa	62	62.441	0.00	Γ_1^+
icsd_614129	BFe_2Ni	62	62.446	0.00	Γ_2^+
icsd_162895	$BiFeO_3$	62	62.448	1.70	Γ_4^+
icsd_004064	Br_3FeK	62	62.441	3.16	Γ_1^+
icsd_075470	Br_3InMn	62	62.446	1.87	Γ_2^+
icsd_042441	Br_3KMn	62	62.446	3.53	Γ_2^+
icsd_035218	$CaMnO_3$	62	62.447	0.53	Γ_3^+

TABLE S53. Tabulated information on **altermagnetic** materials, including the chemical formula, space group, magnetic space group, band gap and corresponding irreducible representations of crystallographic space group.

ICSD number	Chemical formula	SG NUM	BNS	Band Gap (eV)	Irrep
icsd_172790	$CaMoO_3$	62	62.447	0.01	Γ_3^+
icsd_051291	CaO_3Ru	62	62.441	0.50	Γ_1^+
icsd_081056	CaO_3V	62	62.448	0.81	Γ_4^+
icsd_670827	$CCuFe_2$	62	62.447	0.00	Γ_3^+
icsd_670837	CFe_2V	62	62.448	0.00	Γ_4^+
icsd_032710	Cl_3KMn	62	62.441	4.29	Γ_1^+
icsd_023168	Cl_3MnTl	62	62.446	3.77	Γ_2^+
icsd_622489	CoCrP	62	62.441	0.00	Γ_1^+
icsd_622955	CoFeP	62	62.441	0.00	Γ_1^+
icsd_601861	CoGeLu	62	62.446	0.00	Γ_2^+
icsd_052968	CoGeMn	62	62.447	0.00	Γ_3^+
icsd_164459	$CoLaO_3$	62	62.448	1.46	Γ_4^+
icsd_000496	CoO_3Se	62	62.441	3.15	Γ_1^+
icsd_000500	CoO_3Te	62	62.441	2.65	Γ_1^+
icsd_155834	CoO_3Y	62	62.441	1.69	Γ_1^+
icsd_049726	CoPZr	62	62.446	0.00	Γ_2^+
icsd_165245	CoScSi	62	62.447	0.00	Γ_3^+
icsd_625144	CoSiZr	62	62.446	0.00	Γ_2^+
icsd_185586	$CrInO_3$	62	62.441	1.51	Γ_1^+
icsd_009938	$CrLaO_3$	62	62.446	2.37	Γ_2^+
icsd_051123	$CrLaS_3$	62	62.446	0.80	Γ_2^+
icsd_165255	CrNiSi	62	62.446	0.00	Γ_2^+
icsd_085141	CrO_3Sc	62	62.441	2.36	Γ_1^+
icsd_238834	CrO_3Tl	62	62.447	0.27	Γ_3^+
icsd_053283	CuGeTi	62	62.441	0.00	Γ_1^+
icsd_087197	CuSiTi	62	62.447	0.00	Γ_3^+
icsd_068981	F_3FeNa	62	62.446	3.18	Γ_2^+
icsd_031820	F_3KMn	62	62.446	4.01	Γ_2^+
icsd_015621	F_3MnNa	62	62.446	3.74	Γ_2^+
icsd_009008	F_3NaNi	62	62.441	4.85	Γ_1^+
icsd_028255	$FeLaO_3$	62	62.446	2.53	Γ_2^+
icsd_027285	$FeLuO_3$	62	62.446	2.69	Γ_2^+
icsd_632794	FeNbP	62	62.441	0.00	Γ_1^+
icsd_165243	FeNiSi	62	62.441	0.00	Γ_1^+
icsd_093835	FeO_3Tl	62	62.446	0.65	Γ_2^+
icsd_043260	FeO_3Y	62	62.446	2.60	Γ_2^+
icsd_043204	FePZr	62	62.441	0.00	Γ_1^+
icsd_166445	FeSe	62	62.441	0.00	Γ_1^+
icsd_038636	$FNaNbO_2$	62	62.447	0.00	Γ_3^+
icsd_084948	$HMnO_2$	62	62.446	1.61	Γ_2^+
icsd_026420	I_3MnTl	62	62.446	1.96	Γ_2^+
icsd_008146	LaO_3Ti	62	62.441	1.42	Γ_1^+
icsd_063520	LaO_3V	62	62.446	1.70	Γ_2^+
icsd_185830	LuO_3V	62	62.448	1.55	Γ_4^+
icsd_055622	Mn_3Sn_2	62	62.441	0.00	Γ_1^+
icsd_068280	MnNbP	62	62.446	0.00	Γ_2^+
icsd_020228	MnO_2	62	62.447	1.43	Γ_3^+
icsd_000495	MnO_3Se	62	62.448	3.64	Γ_4^+
icsd_158732	MnO_3Ti	62	62.446	2.34	Γ_2^+
icsd_076095	MnPZr	62	62.447	0.00	Γ_3^+
icsd_098405	MoPRu	62	62.446	0.00	Γ_2^+
icsd_000497	NiO_3Se	62	62.446	2.84	Γ_2^+
icsd_646165	NiPTi	62	62.447	0.00	Γ_3^+
icsd_183450	O_3SrTc	62	62.441	1.61	Γ_1^+
icsd_095577	O_3VY	62	62.446	1.95	Γ_2^+
icsd_063228	BaS_3V	63	63.462	0.31	Γ_2^+
icsd_658704	Bi_2Cs_2Ni	63	63.457	0.24	Γ_1^+
icsd_161460	$CCuN_2$	63	63.462	0.77	Γ_2^+
icsd_192148	CoF_3Na	63	63.464	3.96	Γ_4^+
icsd_251575	F_3FeNa	63	63.462	3.34	Γ_2^+
icsd_192141	F_3NaNi	63	63.462	4.90	Γ_2^+
icsd_180910	O_3RuSr	63	63.457	0.48	Γ_1^+
icsd_023265	Mn_2S_4Sn	65	65.486	0.90	Γ_3^+
icsd_670121	$CuMgO_2$	67	67.506	1.29	Γ_3^+
icsd_670124	CuO_2Pb	74	74.558	1.08	Γ_2^+

TABLE S54. Tabulated information on **altermagnetic** materials, including the chemical formula, space group, magnetic space group, band gap and corresponding irreducible representations of crystallographic space group.

ICSD number	Chemical formula	SG NUM	BNS	Band Gap (eV)	Irrep
icsd_174205	MoO_3Sr	74	74.554	0.00	Γ_1^+
icsd_183451	O_3SrTc	74	74.554	1.63	Γ_1^+
icsd_168323	$H_{0.5}Ti$	86	13.69	0.00	$\Gamma_3^+\Gamma_4^+$
icsd_056181	HTi	86	47.252	0.00	$\Gamma_3^+\Gamma_4^+$
icsd_033768	$FeNaO_2$	92	92.113	2.93	Γ_2
icsd_075318	$BBaCuLaO_5$	100	100.174	1.27	Γ_2
icsd_167073	F_6LiMnV	102	102.190	2.64	Γ_2
icsd_246244	$CaFeO_2$	113	18.19	1.61	Γ_5
icsd_291413	$MnMoO_6Te$	113	18.19	2.76	Γ_5
icsd_063423	$Ba_2Cu_3O_6Y$	115	115.285	0.00	Γ_4
icsd_093241	$CuSb_3Ti_2$	115	115.285	0.00	Γ_4
icsd_631756	$FeGa_3$	118	34.158	0.00	Γ_5
icsd_192470	$AgFe_2GaTe_4$	121	121.327	0.89	Γ_1
icsd_160047	$CuFe_2InSe_4$	121	121.327	1.36	Γ_1
icsd_056263	$AgFeS_2$	122	43.226	1.14	Γ_5
icsd_004199	$CoKO_2$	122	24.55	1.72	Γ_5
icsd_430299	$CsOS_2V_2$	123	47.252	0.00	Γ_5^+
icsd_005431	B_2FeMo_2	127	127.387	0.00	Γ_1^+
icsd_614047	B_2FeNb_2	127	55.358	0.00	Γ_5^+
icsd_043016	B_2FeW_2	127	127.387	0.00	Γ_1^+
icsd_107331	Co_2InZr_2	127	127.391	0.00	Γ_2^+
icsd_004054	F_3KMn	127	55.358	3.98	Γ_5^+
icsd_085499	F_4FeRb	127	127.387	3.47	Γ_1^+
icsd_401730	In_5Ti_2	127	127.391	0.00	Γ_2^+
icsd_009167	CoF_2	136	136.499	4.15	Γ_2^+
icsd_407550	$CoIn_3$	136	136.499	0.00	Γ_2^+
icsd_083367	CuO_6Ta_2	136	136.499	1.17	Γ_2^+
icsd_009166	F_2Fe	136	58.398	3.26	Γ_5^+
icsd_009165	F_2Mn	136	136.499	3.59	Γ_2^+
icsd_009168	F_2Ni	136	65.486	4.43	Γ_5^+
icsd_016763	F_2Pd	136	58.398	1.77	Γ_5^+
icsd_032552	F_2V	136	58.398	2.68	Γ_5^+
icsd_165210	F_6Li_2Ru	136	136.499	1.46	Γ_2^+
icsd_201756	F_6Na_2Nb	136	65.486	0.09	Γ_5^+
icsd_633444	Fe_4ScSi_2	136	136.495	0.00	Γ_1^+
icsd_168834	H_2Ti	136	58.398	0.00	Γ_5^+
icsd_000393	MnO_2	136	65.486	0.24	Γ_5^+
icsd_099714	MoO_2	136	136.499	0.00	Γ_2^+
icsd_154021	O_2Re	136	136.499	0.00	Γ_2^+
icsd_015071	O_2Ru	136	136.499	0.00	Γ_2^+
icsd_023600	O_6Ta_2V	136	136.499	0.45	Γ_2^+
icsd_092989	AsTiZr	139	71.536	0.00	Γ_5^+
icsd_186502	$Fe_2Na_2OSe_2$	139	69.524	2.04	Γ_5^+
icsd_248378	$BaIrO_3$	140	140.541	0.00	Γ_1^+
icsd_008000	CuF_3K	140	140.545	2.91	Γ_2^+
icsd_069656	CuF_3Rb	140	69.524	3.04	Γ_5^+
icsd_075412	F_3KMn	140	72.544	3.97	Γ_5^+
icsd_174206	MoO_3Sr	140	72.544	0.00	Γ_5^+
icsd_183452	O_3SrTc	140	140.541	1.66	Γ_1^+
icsd_613476	BCr	141	74.559	0.00	Γ_5^+
icsd_022093	Cl_3Ru	158	9.39	0.36	Γ_3
icsd_246425	$BiCrO_3$	161	161.69	1.85	Γ_1
icsd_015299	$BiFeO_3$	161	9.39	2.25	Γ_3
icsd_252433	LiO_3Os	161	161.69	0.29	Γ_1
icsd_073132	AlF_6LiPd	163	15.89	3.13	Γ_3^+
icsd_078748	$F_6GaLiPd$	163	15.89	3.02	Γ_3^+
icsd_075971	FeN_2W	163	194.268	0.05	Γ_1^+
icsd_034474	$BFeO_3$	167	15.89	2.41	Γ_3^+
icsd_402039	BO_3Ti	167	15.85	2.62	Γ_3^+
icsd_005208	$CCoO_3$	167	167.103	3.26	Γ_1^+
icsd_100678	$CFeO_3$	167	15.85	3.37	Γ_3^+
icsd_028556	$CMnO_3$	167	167.103	4.01	Γ_1^+
icsd_061067	$CNiO_3$	167	15.85	3.45	Γ_3^+
icsd_016672	CoF_3	167	167.103	2.56	Γ_1^+
icsd_025828	CrF_3	167	15.85	2.86	Γ_3^+

TABLE S55. Tabulated information on **altermagnetic** materials, including the chemical formula, space group, magnetic space group, band gap and corresponding irreducible representations of crystallographic space group.

ICSD number	Chemical formula	SG NUM	BNS	Band Gap (eV)	Irrep
icsd_015840	Fe_2O_3	167	167.103	2.31	Γ_1^+
icsd_252432	LiO_3Os	167	167.103	0.28	Γ_1^+
icsd_001462	O_3Ti_2	167	15.85	2.01	Γ_3^+
icsd_192733	$BaCoO_3$	176	63.462	0.00	$\Gamma_3^+\Gamma_5^+$
icsd_002769	$BaFe_2O_4$	182	20.34	3.37	Γ_6
icsd_042687	$FeNb_3S_6$	182	20.31	0.00	Γ_5
icsd_632811	$FeNb_3Se_6$	182	20.31	0.00	Γ_5
icsd_633323	FeS_6Ta_3	182	20.33	0.00	Γ_5
icsd_645098	Nb_3NiSe_6	182	182.182	0.00	Γ_3
icsd_645331	Nb_3S_6Ti	182	20.33	0.21	Γ_5
icsd_645338	Nb_3S_6V	182	20.33	0.00	Γ_5
icsd_645394	Nb_3Se_6Ti	182	182.182	0.19	Γ_3
icsd_042650	$NbS_2V_{0.333}$	182	20.31	0.00	Γ_5
icsd_097539	Ba_3CrS_5	185	36.176	0.00	Γ_5
icsd_022092	Cl_3Ru	185	185.200	0.39	Γ_4
icsd_023873	$BaMnO_3$	186	194.268	1.35	Γ_3
icsd_002590	Br_3CrCs	186	186.205	0.86	Γ_3
icsd_252146	CaCoOS	186	186.205	1.74	Γ_3
icsd_251820	CaFeOS	186	36.172	2.00	Γ_5
icsd_010206	Cl_3CrCs	186	186.205	1.06	Γ_3
icsd_281495	$ClFeN_3O_3$	186	36.172	1.00	Γ_5
icsd_043458	CoO	186	36.172	1.44	Γ_5
icsd_008105	$CrCsI_3$	186	186.205	0.54	Γ_3
icsd_054657	CuSnTi	186	186.205	0.00	Γ_3
icsd_053528	FeS	186	36.176	0.84	Γ_5
icsd_068847	FeS	186	36.176	1.36	Γ_5
icsd_080029	MnN_2W	186	186.205	0.00	Γ_3
icsd_262928	MnO	186	36.172	0.66	Γ_5
icsd_044765	MnS	186	36.172	2.36	Γ_5
icsd_643594	MnSe	186	36.172	1.89	Γ_5
icsd_168369	MoN	186	186.205	0.00	Γ_3
icsd_042493	NiS	186	186.205	0.96	Γ_3
icsd_002536	$BaFe_4O_8Sr$	187	187.211	0.00	Γ_4
icsd_022091	Cl_3Ru	188	40.206	0.36	Γ_5
icsd_413691	Br_3Ru	193	63.462	0.43	Γ_5^+
icsd_004068	Br_3Zr	193	63.462	0.91	Γ_5^+
icsd_240157	Ca_5MnPb_3	193	193.259	0.00	Γ_3^+
icsd_022090	Cl_3Ru	193	193.259	0.38	Γ_3^+
icsd_026069	Cl_3Ti	193	193.259	2.51	Γ_3^+
icsd_023163	Cl_3Zr	193	63.457	1.14	Γ_5^+
icsd_633412	$FeSb_3Zr_5$	193	193.259	0.00	Γ_3^+
icsd_023947	HfI_3	193	193.259	0.03	Γ_3^+
icsd_023172	I_3Ti	193	63.462	1.66	Γ_5^+
icsd_023946	I_3Zr	193	63.462	0.54	Γ_5^+
icsd_080907	La_3Sb_5Ti	193	193.259	0.00	Γ_3^+
icsd_002786	$AgFeO_2$	194	194.268	1.47	Γ_4^+
icsd_057506	AlAuTi	194	63.457	0.00	Γ_5^+
icsd_057984	AlMnPt	194	63.462	0.00	Γ_5^+
icsd_163350	AlPtTi	194	63.462	0.00	Γ_5^+
icsd_044074	AsTi	194	63.457	0.00	Γ_5^+
icsd_670081	$AuCoO_2$	194	63.462	0.00	Γ_5^+
icsd_000922	$BaCoO_3$	194	194.268	1.36	Γ_4^+
icsd_010331	$BaMnO_3$	194	63.462	1.84	Γ_5^+
icsd_084652	BaO_3Ru	194	194.268	0.00	Γ_4^+
icsd_008193	BaS_3V	194	63.462	0.33	Γ_5^+
icsd_106318	Be_2Fe	194	63.462	0.00	Γ_5^+
icsd_616410	Be_2Ru	194	63.462	0.00	Γ_5^+
icsd_174041	Br_3CsFe	194	63.457	3.00	Γ_5^+
icsd_002782	Br_3CsMn	194	63.462	3.74	Γ_5^+
icsd_423829	Br_3CsNi	194	194.268	2.22	Γ_4^+
icsd_041320	Br_3CsTi	194	63.457	2.45	Γ_5^+
icsd_201829	Br_3CsV	194	63.462	3.28	Γ_5^+
icsd_009704	Br_3MnRb	194	194.268	3.45	Γ_4^+
icsd_015011	Br_3NiRb	194	194.268	2.20	Γ_4^+
icsd_154257	Br_3RbTi	194	63.457	2.45	Γ_5^+

TABLE S56. Tabulated information on **altermagnetic** materials, including the chemical formula, space group, magnetic space group, band gap and corresponding irreducible representations of crystallographic space group.

ICSD number	Chemical formula	SG NUM	BNS	Band Gap (eV)	Irrep
icsd_201831	Br_3RbV	194	63.462	3.21	Γ_5^+
icsd_163549	C_3AlV_4	194	63.457	0.00	Γ_5^+
icsd_249387	$CCoN_2$	194	63.457	2.33	Γ_5^+
icsd_419223	$CFeN_2$	194	63.462	2.09	Γ_5^+
icsd_155189	Cl_3CoTl	194	63.462	3.16	Γ_5^+
icsd_036132	Cl_3CrCs	194	194.268	1.09	Γ_4^+
icsd_059371	Cl_3CsNi	194	194.268	3.00	Γ_4^+
icsd_049748	Cl_3CsTi	194	63.462	2.48	Γ_5^+
icsd_015932	Cl_3CsV	194	194.268	3.56	Γ_4^+
icsd_084212	Cl_3CuRb	194	194.268	1.17	Γ_4^+
icsd_015010	Cl_3NiRb	194	194.268	2.94	Γ_4^+
icsd_049747	Cl_3RbTi	194	63.462	2.47	Γ_5^+
icsd_201830	Cl_3RbV	194	63.462	3.50	Γ_5^+
icsd_249388	CN_2Ni	194	194.268	2.10	Γ_4^+
icsd_657109	$Co_{1.82}S_{2.08}$	194	63.462	0.89	Γ_5^+
icsd_624986	$Co_{1.82}Se_{2.08}$	194	63.462	0.07	Γ_5^+
icsd_409451	CoCrGe	194	63.462	0.00	Γ_5^+
icsd_624219	$CoMoP_2$	194	194.268	0.00	Γ_4^+
icsd_624660	CoP_2W	194	194.268	0.00	Γ_4^+
icsd_029305	CoS	194	63.462	0.91	Γ_5^+
icsd_042541	CoSe	194	63.462	0.19	Γ_5^+
icsd_082065	$CrCuO_2$	194	194.268	2.09	Γ_4^+
icsd_158976	$CrGe_3La$	194	194.268	0.00	Γ_4^+
icsd_425293	$CrKO_2$	194	194.268	2.65	Γ_4^+
icsd_053210	CrSb	194	194.268	0.00	Γ_4^+
icsd_010042	CsI_3Mn	194	194.268	2.78	Γ_4^+
icsd_423830	CsI_3Ni	194	63.457	1.26	Γ_5^+
icsd_154258	CsI_3Ti	194	63.457	2.25	Γ_5^+
icsd_026453	CsI_3V	194	63.462	2.81	Γ_5^+
icsd_066546	$CuFeO_2$	194	194.268	1.43	Γ_4^+
icsd_633476	$Fe_{1.82}Se_{2.08}$	194	63.457	1.33	Γ_5^+
icsd_659040	$Fe_{2.85}N_{1.14}$	194	63.462	0.00	Γ_5^+
icsd_081488	FeN_2W	194	63.462	0.00	Γ_5^+
icsd_029302	FeS	194	63.462	0.74	Γ_5^+
icsd_029308	FeSe	194	63.457	1.11	Γ_5^+
icsd_056142	FeTe	194	63.462	0.00	Γ_5^+
icsd_156263	GaPtTi	194	63.462	0.00	Γ_5^+
icsd_103990	$GaTi_2$	194	194.268	0.00	Γ_4^+
icsd_164891	Ge_3LaV	194	63.462	0.00	Γ_5^+
icsd_056288	$HCoO_2$	194	63.457	1.34	Γ_5^+
icsd_191077	HTi	194	63.462	0.00	Γ_5^+
icsd_191079	HV	194	194.268	0.00	Γ_4^+
icsd_081489	$MnMoN_2$	194	63.457	0.54	Γ_5^+
icsd_076218	MnSe	194	63.457	1.00	Γ_5^+
icsd_191172	MnSn	194	63.462	0.00	Γ_5^+
icsd_043541	MnTe	194	194.268	0.49	Γ_4^+
icsd_029313	NiS	194	194.268	0.96	Γ_4^+
icsd_671080	NiSbV	194	63.462	0.00	Γ_5^+
icsd_029310	NiSe	194	63.457	0.00	Γ_5^+
icsd_042557	NiTe	194	63.462	0.00	Γ_5^+
icsd_185562	NRu	194	63.462	0.00	Γ_5^+
icsd_076406	SbTi	194	63.462	0.00	Γ_5^+
icsd_023910	SbV	194	63.462	0.00	Γ_5^+
icsd_083868	SeV	194	194.268	1.59	Γ_4^+
icsd_052121	STi	194	194.268	0.00	Γ_4^+
icsd_033613	SV	194	194.268	0.98	Γ_4^+
icsd_052509	TeV	194	63.462	0.75	Γ_5^+
icsd_053938	AsCoS	198	19.25	0.84	$\Gamma_2\Gamma_3$
icsd_042417	CrGe	198	19.27	0.00	Γ_4
icsd_016837	CrSi	198	19.25	0.00	$\Gamma_2\Gamma_3$
icsd_043054	FeGe	198	19.25	0.00	$\Gamma_2\Gamma_3$
icsd_005250	FeSi	198	19.27	0.00	Γ_4
icsd_633475	$FeSe_2$	205	61.436	0.00	Γ_4^+
icsd_015991	MnS_2	205	61.436	1.08	Γ_4^+
icsd_024020	$MnSe_2$	205	61.436	0.58	Γ_4^+

TABLE S57. Tabulated information on **altermagnetic** materials, including the chemical formula, space group, magnetic space group, band gap and corresponding irreducible representations of crystallographic space group.

ICSD number	Chemical formula	SG NUM	BNS	Band Gap (eV)	Irrep
icsd_646897	$NiTe_2$	205	61.436	0.00	Γ_4^+
icsd_066939	O_2Ru	205	61.436	0.02	Γ_4^+

IV. TOPOLOGICAL MAGNETIC MATERIALS IN OUR MAGNETIC MATERIALS DATABASE

For decades, the topology of electronic band structures has been a central research focus [59–65]. Owing to the development of topological quantum chemistry and symmetry-indicator theory [66–70], tens of thousands of nonmagnetic topological materials have been identified [71–73]. However, due to the limited number of known magnetic structures, theoretical predictions of magnetic topological materials remain relatively scarce, with only a few hundred reported to date [74, 75]. Based on our magnetic structure database, we employ magnetic topological quantum chemistry to identify 1,070 magnetic topological materials [75, 76], substantially expanding the known database of magnetic topological materials.

Among the more than 2,900 magnetic materials contained in our constructed magnetic structure database, we successfully determined the topological classifications of 2,814 materials. Fig. S4 presents a statistical overview of the topological classifications of these magnetic materials. The data are divided into five distinct topological classifications, as defined by the accompanying abbreviations:

The magnetic topological insulating phases (TIs) comprise 125 materials, accounting for 4.4% of the dataset. These include axion insulators (AXIs), three-dimensional quantum anomalous Hall insulators (3D QAHIs), magnetic topological crystalline insulators (TCIs), and higher-order topological insulators (HOTIs). The detailed information of these materials is fully listed in section IV B.

Smith-index semimetals (SISMs) are defined as topological semimetals whose band crossings do not occur at high-symmetry points, lines, or planes, but are instead enforced at generic momenta in the Brillouin zone. We identify 57 SISMs, corresponding to 2.0% of the dataset. Detailed information on these materials is provided in section IV C.

Enforced semimetals with Fermi degeneracy (ESFD) are topological semimetals characterized by degenerate points at high-symmetry points in the Brillouin zone. A total of 85 ESFD are found, accounting for 3.0%. A complete list of detailed information for these materials is presented in section IV D.

Enforced semimetals (ESs) are topological semimetals in which band crossings occur along high-symmetry lines or planes due to the violation of compatibility relations. We identify 803 ESs, representing 28.5% of the dataset. The complete details of these materials are presented in section IV E.

Linear combinations of elementary band representations (LCEBR) indicate the absence of symmetry-protected topological features and comprise 1744 entries, accounting for 61.9% of the total dataset. Further details of these materials can be found in section IV F.

The magnetic structure, electronic band structures, and associated information of topological magnetic materials is available at `https://magdatabase.nju.edu.cn`, which is continuously updated.

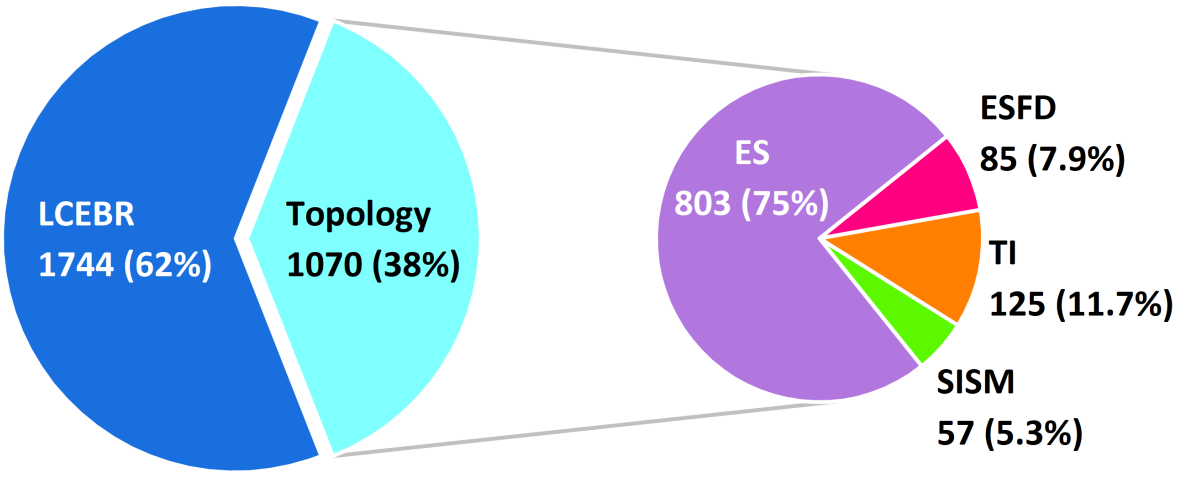


FIG. S4. Statistics of Topological Classification.

A. Representative Materials of Magnetic Topological Semimetals

In the main text, we present three representative magnetic topological semimetals: V_3Ga_2 (icsd_635637), MnTe (icsd_076241), and Co_3SnC (icsd_108129).

The paramagnetic phase of V_3Ga_2 (icsd_635637) crystallizes in the space group $P4_132$ (No. 213) [77]. Its magnetic structure adopts a noncollinear AFM configuration, as illustrated in Fig. S5(a), corresponding to the magnetic space group $R32$ (155.45). As shown in Fig. S5(b), a Weyl point protected by C_{2x} symmetry appears along the high-symmetry line Γ–F, accompanied by two additional Weyl points protected by C_{3z} symmetry along the T–Γ line. The full distribution of these band-crossing points within the Brillouin zone is presented in Fig. S5. In total, V_3Ga_2 hosts 28 Weyl points throughout the Brillouin zone, with energies spanning from -7 to 28 meV.

The paramagnetic phase of MnTe (icsd_076241) crystallizes in the space group $Pnma$ (No. 62) [78], which corresponds to the high-pressure structure of the altermagnet α-MnTe [79, 80]. Under high pressure, α-MnTe undergoes a structural phase transition from the NiAs-type to the MnP-type structure [78]. Our analysis reveals that MnTe (icsd_076241) adopts a PT AFM configuration, belonging to the magnetic space group $Pn'm'a'$ (62.449), as shown in Fig. S5(d). The band structure exhibits Dirac points along two distinct high-symmetry lines: two Dirac points are located along $k_y = 0$ and $k_z = \pi$, while four additional Dirac points appear along $k_y = \pi$ and $k_z = 0$, as illustrated in Figs. S5(e) and (f).

Co_3SnC (icsd_108129) crystallizes in the antiperovskite structure with space group $Pm\bar{3}m$ (No. 221) [81]. Its magnetic configuration is FM with magnetization oriented along the [001] direction, as shown in Fig. S5(g). Two nodal rings, protected by m_z mirror symmetry, emerge on the high-symmetry planes $k_z = 0$ and $k_z = \pi$. In the calculated band structure in Fig. S5(h), the band crossings associated with the nodal ring on the $k_z = 0$ plane appear along the high-symmetry line X-M, whereas those of the nodal ring on the $k_z = \pi$ plane lie along the A–Z line. Furthermore, 16 Weyl points are found at generic momenta within the Brillouin zone. Taken together, Co_3SnC is identified as a topological semimetal exhibiting the coexistence of nodal rings and Weyl points, as illustrated in Fig. S5(i).

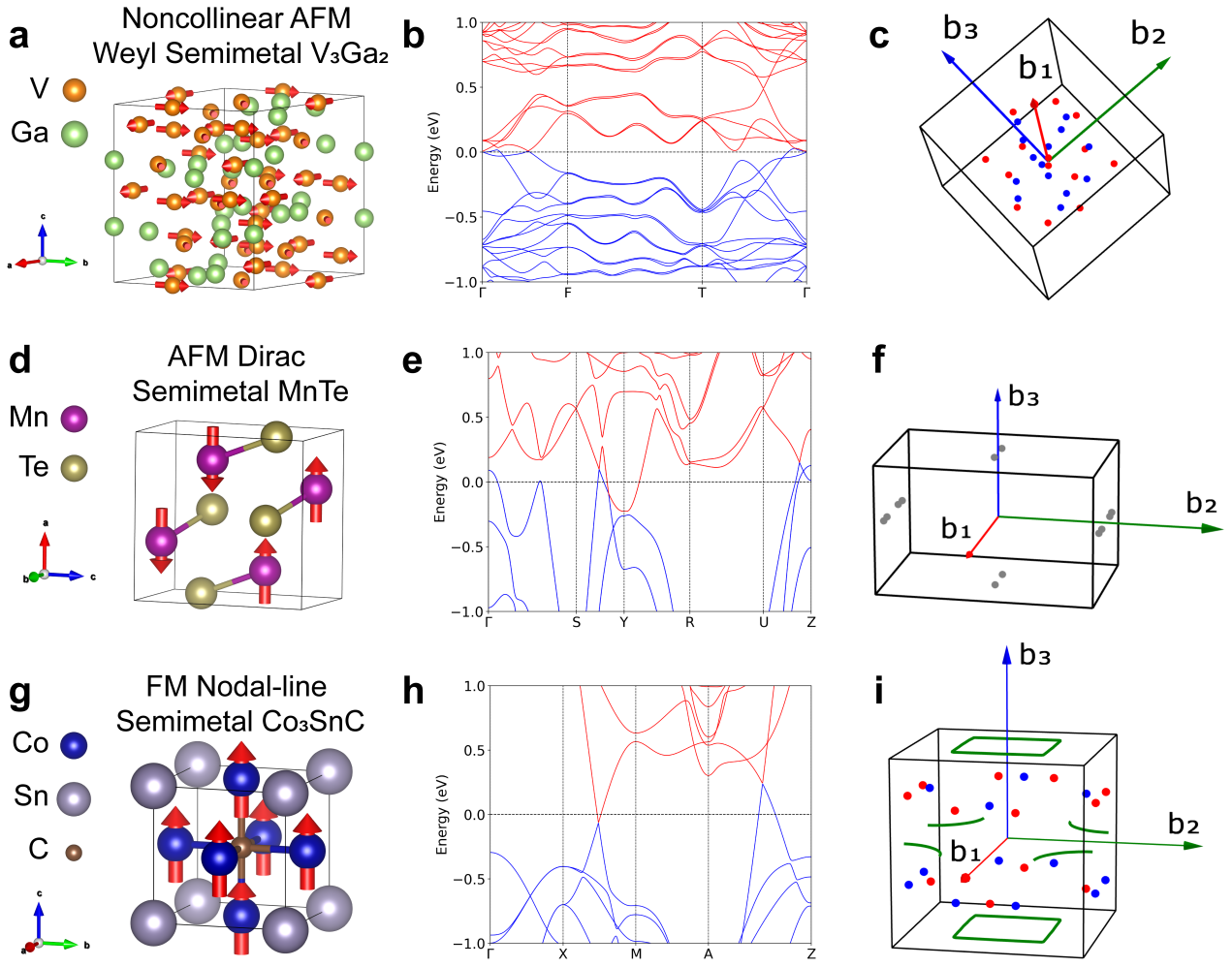


FIG. S5. Topological magnetic semimetals. (a)-(c) Magnetic structure, band structure, and distribution of Weyl points of the non-collinear AFM Weyl semimetal V_3Ga_2. The magnetic moments of V lie in the xy plane, as indicated by red arrow. (d)-(f) Magnetic structure, band structure, and distribution of Dirac points of the AFM Dirac semimetal MnTe. (g)-(i) Magnetic structure, band structure, and distribution of nodal rings and Weyl points of the FM nodal-line semimetal Co_3SnC. The red and blue dots in (c) and (k) denote Weyl points with topological charges $+1$ and -1, respectively, while the green lines represent the nodal rings.

B. Table of Magnetic Topological Insulators

In this subsection, we summarize all magnetic topological insulating phases (TIs) in a series of tables. These tables list the ICSD numbers, chemical formulas, MSGs, symmetry indicators, and topological subclassification. The symmetry indicators adopted here follow the conventions established in Refs. [75, 76]. The possible topological subclassifications include axion insulators (AXIs), three-dimensional quantum anomalous Hall insulators (3D QAHIs), magnetic topological crystalline insulators (TCIs), higher-order topological insulators (HOTIs). Notably, some symmetry indicators cannot uniquely determine the topological subclassifications. For example, $(\eta_{4I}, z_{2I,1}, z_{2I,2}, z_{2I,3}) = (2, 0, 0, 0)$ may correspond either to an AXI or to a high-Chern-number 3D QAHI. In such cases, further calculation of topological invariants is required to confirm the subclassification. We separate the possible topological subclassification with a slash ("/").

TABLE S58. ICSD numbers, chemical formulas, magnetic space groups (MSGs), symmetry indicators, and topological subclassifications for magnetic topological insulating phases (TI).

ICSD	Formula	MSG	Symmetry indicators	Topological subclassification
icsd_015079	B_4Mn	12.62	$\eta_{4I} = 0; z_{2I,1} = 1; z_{2I,2} = 1$ $z_{2I,3} = 0$	3D QAHI
icsd_066509	$Cu_2Li_3O_4$	12.62	$\eta_{4I} = 0; z_{2I,1} = 1; z_{2I,2} = 1$ $z_{2I,3} = 1$	3D QAHI
icsd_075420	CrS_2	12.62	$\eta_{4I} = 2; z_{2I,1} = 0; z_{2I,2} = 0$ $z_{2I,3} = 1$	3D QAHI
icsd_251718	$CrSe_2$	12.62	$\eta_{4I} = 2; z_{2I,1} = 0; z_{2I,2} = 0$ $z_{2I,3} = 1$	3D QAHI
icsd_646533	$NiSe_4Si_2$	12.62	$\eta_{4I} = 2; z_{2I,1} = 1; z_{2I,2} = 1$ $z_{2I,3} = 0$	3D QAHI
icsd_169074	As_2BaOTi_2	65.486	$\eta_{4I} = 2; z_{2I,1} = 0; z_{2I,2} = 0$ $\delta_{2m} = 1; z^{-}_{2m,\pi} = 0; z^{+}_{2m,\pi} = 0$	AXI/3D QAHI/TCI
icsd_094745	$ClMnO_3Sr_2$	129.417	$\eta_{4I} = 0; z_{2I,3} = 0; z_{2R} = 0$ $z_{4R} = 2; z_2 = 0; z_{4S} = 2$	3D QAHI
icsd_069044	CaNNi	66.496	$\eta_{4I} = 2; z_{2I,1} = 1; z_{2I,2} = 1$	3D QAHI
icsd_187709	NTc	66.496	$\eta_{4I} = 2; z_{2I,1} = 1; z_{2I,2} = 1$	3D QAHI
icsd_407550	$CoIn_3$	136.499	$\eta_{4I} = 2; \delta_{2m} = 1$	AXI/TCI
icsd_010462	$CaCo_2P_2$	139.536	$z_2 = 1$	AXI
icsd_430064	$Bi_2F_2OSr_2Ti_2$	139.534	$\eta_{4I} = 0; \delta_{2m} = 0; z_4 = 2$	TCI/HOTI
icsd_042531	BCo_2	72.544	$\eta_{4I} = 0; z_{2I,1} = 1; z_{2I,2} = 1$ $z_{2I,3} = 1; \eta'_{2I} = 0; z'_{2R} = 1$	3D QAHI
icsd_062157	$BaMo_6S_8$	2.4	$\eta_{4I} = 2; z_{2I,1} = 0; z_{2I,2} = 0$ $z_{2I,3} = 0$	AXI/3D QAHI
icsd_639106	$HgMo_6S_8$	2.4	$\eta_{4I} = 2; z_{2I,1} = 0; z_{2I,2} = 0$ $z_{2I,3} = 0$	AXI/3D QAHI
icsd_641241	KMo_6S_8	148.17	$\eta_{4I} = 0; z_{2I,1} = 1; z_{2I,2} = 1$ $z_{2I,3} = 1$	3D QAHI
icsd_671511	$AsInNi_3$	2.4	$\eta_{4I} = 2; z_{2I,1} = 0; z_{2I,2} = 0$ $z_{2I,3} = 1$	3D QAHI
icsd_169980	$HNiO_2$	156.51	$z_{3R} = 2$	3D QAHI
icsd_044612	Fe_2N	162.77	$\eta_{4I} = 0; z_{2I,3} = 1; z_{3R} = 0$	3D QAHI
icsd_042559	$NiTe_2$	164.89	$\eta_{4I} = 2; z_{2I,3} = 0; z_{3R} = 0$	AXI/3D QAHI
icsd_603582	Te_2V	12.62	$\eta_{4I} = 0; z_{2I,1} = 0; z_{2I,2} = 0$ $z_{2I,3} = 1$	3D QAHI
icsd_001004	ClSc	166.101	$\eta_{4I} = 0; z_{2I,1} = 1; z_{2I,2} = 1$ $z_{2I,3} = 1$	3D QAHI
icsd_005435	$Co_3S_2Sn_2$	12.62	$\eta_{4I} = 2; z_{2I,1} = 0; z_{2I,2} = 0$ $z_{2I,3} = 1$	3D QAHI
icsd_108894	$In_2Ni_3S_2$	12.58	$\eta_{4I} = 2; z_{2I,1} = 0; z_{2I,2} = 0$ $\delta_{2m} = 1; z^{-}_{2m,\pi} = 0; z^{+}_{2m,\pi} = 0$	AXI/3D QAHI/TCI
icsd_168949	CoY	12.62	$\eta_{4I} = 2; z_{2I,1} = 0; z_{2I,2} = 0$ $z_{2I,3} = 1$	3D QAHI
icsd_425966	Bi_2MnTe_4	166.101	$\eta_{4I} = 2; z_{2I,1} = 0; z_{2I,2} = 0$ $z_{2I,3} = 0$	AXI/3D QAHI
icsd_670141	$CrGa_4$	12.62	$\eta_{4I} = 2; z_{2I,1} = 0; z_{2I,2} = 0$ $z_{2I,3} = 0$	AXI/3D QAHI
icsd_670405	Fe_6Ge_4Mg	166.101	$\eta_{4I} = 3; z_{2I,1} = 1; z_{2I,2} = 1$ $z_{2I,3} = 1$	3D QAHI
icsd_182148	Sn_6V_6Y	65.486	$\eta_{4I} = 2; z_{2I,1} = 0; z_{2I,2} = 0$ $\delta_{2m} = 1; z^{-}_{2m,\pi} = 0; z^{+}_{2m,\pi} = 0$	AXI/3D QAHI/TCI
icsd_023910	SbV	63.462	$\eta_{4I} = 2$	AXI/3D QAHI
icsd_042557	NiTe	63.462	$\eta_{4I} = 2$	AXI/3D QAHI
icsd_044074	AsTi	63.457	$\eta_{4I} = 2; \delta_{2m} = 1$	AXI/TCI
icsd_056142	FeTe	63.462	$\eta_{4I} = 2$	AXI/3D QAHI
icsd_057506	AlAuTi	63.457	$\eta_{4I} = 2; \delta_{2m} = 1$	AXI/TCI

TABLE S59. ICSD numbers, chemical formulas, magnetic space groups (MSGs), symmetry indicators, and topological subclassifications for magnetic topological insulating phases (TI).

ICSD	Formula	MSG	Symmetry indicators	Topological subclassification
icsd_076118	CoSb	63.463	$\eta_{4I}=2; z_{2I,1}=0; z_{2I,2}=0$ $\delta_{2m}=1; z^{-}_{2m,\pi}=0; z^{+}_{2m,\pi}=0$	AXI/3D QAHI/TCI
icsd_076406	SbTi	63.462	$\eta_{4I}=2$	AXI/3D QAHI
icsd_169821	NV	63.464	$\eta_{4I}=2; z_{2I,1}=0; z_{2I,2}=0$ $\eta'_{2I}=1; z'_{2R}=0$	AXI/3D QAHI
icsd_603343	$GeMn_3$	63.464	$\eta_{4I}=2; z_{2I,1}=0; z_{2I,2}=0$ $\eta'_{2I}=1; z'_{2R}=0$	AXI/3D QAHI
icsd_616410	Be_2Ru	63.462	$\eta_{4I}=2$	AXI/3D QAHI
icsd_077829	LaSe	2.4	$\eta_{4I}=0; z_{2I,1}=0; z_{2I,2}=0$ $z_{2I,3}=1$	3D QAHI
icsd_633475	$FeSe_2$	61.436	$\eta_{4I}=2$	AXI/3D QAHI
icsd_633869	$FeTe_2$	61.433	$\eta_{4I}=2$	AXI
icsd_646897	$NiTe_2$	61.436	$\eta_{4I}=2$	AXI/3D QAHI
icsd_044729	CFe_4	111.255	$z_{2R}=0; \delta_{2S}=0; z_2=1$ $z_{4S}=0$	AXI/3D QAHI
icsd_023586	$CGaMn_3$	166.101	$\eta_{4I}=0; z_{2I,1}=1; z_{2I,2}=1$ $z_{2I,3}=1$	3D QAHI
icsd_052642	$AlNTi_3$	65.486	$\eta_{4I}=2; z_{2I,1}=1; z_{2I,2}=1$ $\delta_{2m}=1; z^{-}_{2m,\pi}=1; z^{+}_{2m,\pi}=1$	3D QAHI/TCI
icsd_057928	AlIr	123.345	$\delta_{4m}=2; z^{-}_{4m,\pi}=2; z^{+}_{4m,\pi}=2$	TCI
icsd_058726	BeNi	65.486	$\eta_{4I}=2; z_{2I,1}=0; z_{2I,2}=0$ $\delta_{2m}=1; z^{-}_{2m,\pi}=0; z^{+}_{2m,\pi}=0$	AXI/3D QAHI/TCI
icsd_058728	BePd	65.486	$\eta_{4I}=2; z_{2I,1}=0; z_{2I,2}=0$ $\delta_{2m}=1; z^{-}_{2m,\pi}=0; z^{+}_{2m,\pi}=0$	AXI/3D QAHI/TCI
icsd_096119	Mn_3Sb	166.101	$\eta_{4I}=2; z_{2I,1}=1; z_{2I,2}=1$ $z_{2I,3}=1$	3D QAHI
icsd_168838	$H_2Mg_{0.75}Ti_{0.25}$	65.486	$\eta_{4I}=2; z_{2I,1}=0; z_{2I,2}=0$ $\delta_{2m}=1; z^{-}_{2m,\pi}=0; z^{+}_{2m,\pi}=0$	AXI/3D QAHI/TCI
icsd_187256	MgNi	166.101	$\eta_{4I}=2; z_{2I,1}=0; z_{2I,2}=0$ $z_{2I,3}=0$	AXI/3D QAHI
icsd_052330	SbV_3	223.106	$z_2=1$	AXI
icsd_026630	H_2Cr	166.101	$\eta_{4I}=2; z_{2I,1}=0; z_{2I,2}=0$ $z_{2I,3}=0$	AXI/3D QAHI
icsd_057008	CCr	166.101	$\eta_{4I}=2; z_{2I,1}=0; z_{2I,2}=0$ $z_{2I,3}=0$	AXI/3D QAHI
icsd_180457	CNi	71.536	$\eta_{4I}=2; z_{2I,1}=0; z_{2I,2}=0$ $z_{2I,3}=0; \delta_{2m}=1; z^{-}_{2m,\pi}=0$ $z^{+}_{2m,\pi}=0$	AXI/3D QAHI/TCI
icsd_086427	CuO_5Sr_2Tl	47.252	$\delta_{2m}=0; z^{-}_{2m,\pi}=1; z^{+}_{2m,\pi}=1$	TCI
icsd_041726	$CrSb_2$	58.398	$\eta_{4I}=2$	AXI/3D QAHI
icsd_169570	NiS_2	58.398	$\eta_{4I}=2$	AXI/3D QAHI
icsd_196424	B_4Fe	58.398	$\eta_{4I}=2$	AXI/3D QAHI
icsd_166445	FeSe	62.441	$\eta_{4I}=2$	AXI
icsd_168323	$H_{0.5}Ti$	13.69	$\eta_{4I}=0; z_{2I,1}=1; z_{2I,2}=1$	3D QAHI
icsd_084827	$CoHf_2P$	11.54	$\eta_{4I}=2; z_{2I,1}=0; z_{2I,3}=0$	AXI/3D QAHI
icsd_172559	Ag_2NiO_2	12.58	$\eta_{4I}=2; z_{2I,1}=0; z_{2I,2}=0$ $\delta_{2m}=1; z^{-}_{2m,\pi}=0; z^{+}_{2m,\pi}=0$	AXI/3D QAHI/TCI
icsd_617514	$C_3Cr_2Lu_2$	12.62	$\eta_{4I}=0; z_{2I,1}=0; z_{2I,2}=0$ $z_{2I,3}=1$	3D QAHI
icsd_617562	$C_3Cr_2Y_2$	12.62	$\eta_{4I}=0; z_{2I,1}=0; z_{2I,2}=0$ $z_{2I,3}=1$	3D QAHI
icsd_670103	$AuCuO_2$	12.62	$\eta_{4I}=2; z_{2I,1}=1; z_{2I,2}=1$ $z_{2I,3}=0$	3D QAHI
icsd_049726	CoPZr	62.446	$\eta_{4I}=2$	AXI/3D QAHI
icsd_068280	MnNbP	62.446	$\eta_{4I}=2$	AXI/3D QAHI
icsd_076095	MnPZr	62.447	$\eta_{4I}=2$	AXI/3D QAHI
icsd_085947	MnPTa	62.446	$\eta_{4I}=2$	AXI/3D QAHI
icsd_165245	CoScSi	62.447	$\eta_{4I}=2$	AXI/3D QAHI
icsd_614256	BFeW	62.446	$\eta_{4I}=2$	AXI/3D QAHI
icsd_632129	FeGeTa	62.446	$\eta_{4I}=2$	AXI/3D QAHI
icsd_416513	$CoPd_2Se_2$	72.544	$\eta_{4I}=0; z_{2I,1}=1; z_{2I,2}=1$ $z_{2I,3}=1; \eta'_{2I}=0; z'_{2R}=1$	3D QAHI
icsd_600147	$FeGa_8Lu_2$	47.252	$\eta_{4I}=0; z_{2I,3}=0; z_{2R}=0$ $\delta_{2m}=0; z^{-}_{2m,\pi}=1; z^{+}_{2m,\pi}=1$	TCI
icsd_044449	B_2MnW_2	55.358	$\eta_{4I}=2$	AXI/3D QAHI

TABLE S60. ICSD numbers, chemical formulas, magnetic space groups (MSGs), symmetry indicators, and topological subclassifications for magnetic topological insulating phases (TI).

ICSD	Formula	MSG	Symmetry indicators	Topological subclassification
icsd_107331	Co_2InZr_2	127.391	$\eta_{4I}=0;\delta_{2m}=0;z^{-}_{2m,\pi}=0$ $z^{+}_{2m,\pi}=0;z_{2w,3}=0;z_4=2$	TCI
icsd_614047	B_2FeNb_2	55.358	$\eta_{4I}=2$	AXI/3D QAHI
icsd_614207	B_2FeTa_2	55.358	$\eta_{4I}=2$	AXI/3D QAHI
icsd_062598	C_2CoSc	129.417	$\eta_{4I}=2;z_{2I,3}=0;z_{2R}=0$ $z_{4R}=0;z_2=1;z_{4S}=0$	AXI
icsd_085283	CBNiY	59.41	$\eta_{4I}=2$	AXI/3D QAHI
icsd_191258	CrN_3Nb	129.417	$\eta_{4I}=2;z_{2I,3}=1;z_{2R}=1$ $z_{4R}=3;z_2=1;z_{4S}=3$	3D QAHI
icsd_031916	CoO_2Pt	12.58	$\eta_{4I}=2;z_{2I,1}=0;z_{2I,2}=0$ $\delta_{2m}=1;z^{-}_{2m,\pi}=0;z^{+}_{2m,\pi}=0$	AXI/3D QAHI/TCI
icsd_031917	CoO_2Pd	12.62	$\eta_{4I}=2;z_{2I,1}=0;z_{2I,2}=0$ $z_{2I,3}=0$	AXI/3D QAHI
icsd_160574	Ag_2NiO_2	12.58	$\eta_{4I}=2;z_{2I,1}=0;z_{2I,2}=0$ $\delta_{2m}=1;z^{-}_{2m,\pi}=0;z^{+}_{2m,\pi}=0$	AXI/3D QAHI/TCI
icsd_173362	Bi_5La_3Mn	63.464	$\eta_{4I}=0;z_{2I,1}=1;z_{2I,2}=1$ $\eta'_{2I}=0;z_{2R}=1$	3D QAHI
icsd_053018	Co_3Nb_2Si	63.464	$\eta_{4I}=2;z_{2I,1}=0;z_{2I,2}=0$ $\eta'_{2I}=1;z'_{2R}=0$	AXI/3D QAHI
icsd_010509	$Al_{11}Mn_4$	2.4	$\eta_{4I}=2;z_{2I,1}=0;z_{2I,2}=1$ $z_{2I,3}=0$	AXI/3D QAHI
icsd_015214	$NiRh_2Se_4$	12.62	$\eta_{4I}=2;z_{2I,1}=1;z_{2I,2}=1$ $z_{2I,3}=1$	3D QAHI
icsd_023970	$NiSe_4V_2$	12.62	$\eta_{4I}=2;z_{2I,1}=1;z_{2I,2}=1$ $z_{2I,3}=1$	3D QAHI
icsd_035140	NiS_4V_2	12.62	$\eta_{4I}=2;z_{2I,1}=1;z_{2I,2}=1$ $z_{2I,3}=1$	3D QAHI
icsd_038369	$Te_2V_{1.04}$	12.58	$\eta_{4I}=2;z_{2I,1}=1;z_{2I,2}=1$ $\delta_{2m}=1;z^{-}_{2m,\pi}=1;z^{+}_{2m,\pi}=1$	3D QAHI/TCI
icsd_042558	Ni_3Se_4	12.62	$\eta_{4I}=2;z_{2I,1}=1;z_{2I,2}=1$ $z_{2I,3}=0$	3D QAHI
icsd_042563	FeS_4Ti_2	12.62	$\eta_{4I}=2;z_{2I,1}=1;z_{2I,2}=1$ $z_{2I,3}=0$	3D QAHI
icsd_603354	$FeRh_2Se_4$	12.58	$\eta_{4I}=0;z_{2I,1}=1;z_{2I,2}=1$ $\delta_{2m}=0;z^{-}_{2m,\pi}=1;z^{+}_{2m,\pi}=1$	3D QAHI/TCI
icsd_622979	$CoFe_2Se_4$	12.62	$\eta_{4I}=0;z_{2I,1}=0;z_{2I,2}=0$ $z_{2I,3}=1$	3D QAHI
icsd_624485	Co_2NiSe_4	12.62	$\eta_{4I}=2;z_{2I,1}=1;z_{2I,2}=1$ $z_{2I,3}=0$	3D QAHI
icsd_624874	CoS_4Ti_2	12.62	$\eta_{4I}=2;z_{2I,1}=1;z_{2I,2}=1$ $z_{2I,3}=1$	3D QAHI
icsd_625002	$CoSe_4Ti_2$	12.62	$\eta_{4I}=2;z_{2I,1}=1;z_{2I,2}=1$ $z_{2I,3}=1$	3D QAHI
icsd_626577	$CrRh_2Se_4$	12.62	$\eta_{4I}=2;z_{2I,1}=0;z_{2I,2}=0$ $z_{2I,3}=1$	3D QAHI
icsd_633332	$Fe_{0.5}S_2Ti$	12.62	$\eta_{4I}=2;z_{2I,1}=1;z_{2I,2}=1$ $z_{2I,3}=0$	3D QAHI
icsd_085291	$Ba_2Cu_3LaO_8$	47.252	$\eta_{4I}=2;z_{2I,3}=1;z_{2R}=1$ $\delta_{2m}=1;z^{-}_{2m,\pi}=1;z^{+}_{2m,\pi}=0$	3D QAHI/TCI
icsd_615019	B_2Ni_2Sr	58.398	$\eta_{4I}=2$	AXI/3D QAHI
icsd_044339	BCo_3	62.446	$\eta_{4I}=2$	AXI/3D QAHI
icsd_167127	CFe_2Ni	62.446	$\eta_{4I}=2$	AXI/3D QAHI
icsd_251180	CMn_3	62.446	$\eta_{4I}=2$	AXI/3D QAHI
icsd_636746	GeIrTi	62.446	$\eta_{4I}=2$	AXI/3D QAHI
icsd_641017	IrSiTi	62.447	$\eta_{4I}=2$	AXI/3D QAHI
icsd_670822	CCo_2Fe	62.446	$\eta_{4I}=2$	AXI/3D QAHI
icsd_670824	CCr_2Fe	62.446	$\eta_{4I}=2$	AXI/3D QAHI
icsd_670825	$CCrFe_2$	62.441	$\eta_{4I}=2$	AXI
icsd_670827	$CCuFe_2$	62.447	$\eta_{4I}=2$	AXI/3D QAHI
icsd_052332	Sb_4V_5	12.62	$\eta_{4I}=2;z_{2I,1}=0;z_{2I,2}=0$ $z_{2I,3}=0$	AXI/3D QAHI
icsd_614755	B_2MnMo_2	55.358	$\eta_{4I}=2$	AXI/3D QAHI
icsd_091199	$CuMnO_3SSr_2$	129.417	$\eta_{4I}=2;z_{2I,3}=1;z_{2R}=1$ $z_{4R}=3;z_2=1;z_{4S}=3$	3D QAHI

TABLE S61. ICSD numbers, chemical formulas, magnetic space groups (MSGs), symmetry indicators, and topological subclassifications for magnetic topological insulating phases (TI).

ICSD	Formula	MSG	Symmetry indicators	Topological subclassification
icsd_610777	As_2LaRh_2	129.417	$\eta_{4I}=0; z_{2I,3}=1; z_{2R}=1$ $z_{4R}=3; z_2=0; z_{4S}=3$	3D QAHI
icsd_163549	C_3AlV_4	63.457	$\eta_{4I}=2; \delta_{2m}=1$	AXI/TCI
icsd_671080	NiSbV	63.462	$\eta_{4I}=2$	AXI/3D QAHI
icsd_076056	Mn_3NNi	166.101	$\eta_{4I}=2; z_{2I,1}=0; z_{2I,2}=0$ $z_{2I,3}=0$	AXI/3D QAHI
icsd_076060	Mn_3NRh	166.101	$\eta_{4I}=2; z_{2I,1}=0; z_{2I,2}=0$ $z_{2I,3}=0$	AXI/3D QAHI
icsd_052989	Co_2GeTi	71.536	$\eta_{4I}=2; z_{2I,1}=0; z_{2I,2}=0$ $z_{2I,3}=0; \delta_{2m}=1; z^-_{2m,\pi}=0$ $z^+_{2m,\pi}=0$	AXI/3D QAHI/TCI
icsd_057643	$AlCo_2V$	166.101	$\eta_{4I}=2; z_{2I,1}=0; z_{2I,2}=0$ $z_{2I,3}=0$	AXI/3D QAHI
icsd_057994	$AlMn_2V$	166.101	$\eta_{4I}=2; z_{2I,1}=0; z_{2I,2}=0$ $z_{2I,3}=0$	AXI/3D QAHI
icsd_185936	Co_2FeGe	71.536	$\eta_{4I}=2; z_{2I,1}=0; z_{2I,2}=0$ $z_{2I,3}=0; \delta_{2m}=1; z^-_{2m,\pi}=0$ $z^+_{2m,\pi}=0$	AXI/3D QAHI/TCI

C. Table of Magnetic Smith-Index Semimetals

Smith-index semimetals (SISMs) are topological semimetals whose band representations satisfy the compatibility relations, while their symmetry indicators are incompatible with any insulating phase. Consequently, the electronic structure is gapped at all high-symmetry points, lines, and planes, and gapless band crossings are enforced at generic momenta.

In this subsection, we summarize all magnetic SISMs in a series of tables. These tables list the ICSD numbers, chemical formulas, MSGs, symmetry indicators. The symmetry indicators adopted here follow the conventions established in Refs. [75, 76].

TABLE S62. ICSD numbers, chemical formulas, magnetic space groups (MSGs), and symmetry indicators for magnetic Smith-index semimetals (SISM).

ICSD	Formula	MSG	Symmetry indicators
icsd_018176	CoO_4S	11.54	$\eta_{4I}=1; z_{2I,1}=0; z_{2I,3}=0$
icsd_099894	CoO_3Sr_2	12.62	$\eta_{4I}=3; z_{2I,1}=0; z_{2I,2}=0; z_{2I,3}=0$
icsd_624999	$CoSe_4Si_2$	12.62	$\eta_{4I}=3; z_{2I,1}=0; z_{2I,2}=0; z_{2I,3}=0$
icsd_246938	$BaCoS_2$	13.69	$\eta_{4I}=1; z_{2I,1}=1; z_{2I,2}=0$
icsd_062156	Mo_6S_8Sr	148.17	$\eta_{4I}=1; z_{2I,1}=1; z_{2I,2}=1; z_{2I,3}=1$
icsd_237739	Au_5MnY_3	148.17	$\eta_{4I}=1; z_{2I,1}=1; z_{2I,2}=1; z_{2I,3}=1$
icsd_075962	$D_{12}Ba_3Ir_2$	12.62	$\eta_{4I}=1; z_{2I,1}=0; z_{2I,2}=0; z_{2I,3}=0$
icsd_079991	$D_8BaFeMg_2$	12.62	$\eta_{4I}=3; z_{2I,1}=0; z_{2I,2}=0; z_{2I,3}=1$
icsd_086197	D_2CoO_2	12.62	$\eta_{4I}=3; z_{2I,1}=0; z_{2I,2}=0; z_{2I,3}=0$
icsd_626718	$CrSe_2$	12.62	$\eta_{4I}=3; z_{2I,1}=0; z_{2I,2}=0; z_{2I,3}=0$
icsd_420728	$Rh_3S_2Sn_2$	166.101	$\eta_{4I}=3; z_{2I,1}=0; z_{2I,2}=0; z_{2I,3}=0$
icsd_053564	Fe_3Te_3Tl	11.54	$\eta_{4I}=1; z_{2I,1}=0; z_{2I,3}=1$
icsd_080771	Ba_3MnN_3	11.54	$\eta_{4I}=3; z_{2I,1}=0; z_{2I,3}=0$
icsd_000316	FeS_2	148.17	$\eta_{4I}=1; z_{2I,1}=0; z_{2I,2}=0; z_{2I,3}=0$
icsd_191175	MnSb	119.319	$\delta_{2S}=1; z_2=0; z_{4S}=2$
icsd_077036	$CInMn_3$	166.101	$\eta_{4I}=3; z_{2I,1}=0; z_{2I,2}=0; z_{2I,3}=0$
icsd_160196	CrO_3Pb	166.101	$\eta_{4I}=3; z_{2I,1}=0; z_{2I,2}=0; z_{2I,3}=0$
icsd_181144	NZr	166.101	$\eta_{4I}=1; z_{2I,1}=0; z_{2I,2}=0; z_{2I,3}=0$
icsd_236827	MnN	166.101	$\eta_{4I}=3; z_{2I,1}=0; z_{2I,2}=0; z_{2I,3}=0$
icsd_236829	FeN	166.101	$\eta_{4I}=3; z_{2I,1}=0; z_{2I,2}=0; z_{2I,3}=0$
icsd_043356	$SbTi_3$	167.107	$\eta_{4I}=3$
icsd_611501	$AsTi_3$	167.107	$\eta_{4I}=3$
icsd_056182	H_2Ti	166.101	$\eta_{4I}=3; z_{2I,1}=0; z_{2I,2}=0; z_{2I,3}=0$
icsd_096297	D_2Ti	166.101	$\eta_{4I}=3; z_{2I,1}=0; z_{2I,2}=0; z_{2I,3}=0$
icsd_424636	Ga_4Mn	166.101	$\eta_{4I}=3; z_{2I,1}=0; z_{2I,2}=0; z_{2I,3}=0$
icsd_611737	Au_4Cr	12.62	$\eta_{4I}=3; z_{2I,1}=1; z_{2I,2}=1; z_{2I,3}=0$
icsd_014026	$Cr_{0.5}NbSe_2$	12.62	$\eta_{4I}=1; z_{2I,1}=1; z_{2I,2}=1; z_{2I,3}=0$
icsd_645395	Nb_2Se_4Ti	12.62	$\eta_{4I}=1; z_{2I,1}=1; z_{2I,2}=1; z_{2I,3}=0$
icsd_100785	$LaRu_3Si_2$	11.54	$\eta_{4I}=1; z_{2I,1}=0; z_{2I,3}=0$
icsd_040908	MnPdTe	119.319	$\delta_{2S}=1; z_2=0; z_{4S}=0$
icsd_052673	AuMnSb	119.319	$\delta_{2S}=1; z_2=0; z_{4S}=0$
icsd_057504	$AlAu_2Mn$	166.101	$\eta_{4I}=3; z_{2I,1}=0; z_{2I,2}=0; z_{2I,3}=0$
icsd_057981	$AlMnPd_2$	166.101	$\eta_{4I}=1; z_{2I,1}=0; z_{2I,2}=0; z_{2I,3}=0$
icsd_001501	O_2V	2.4	$\eta_{4I}=3; z_{2I,1}=0; z_{2I,2}=0; z_{2I,3}=1$
icsd_159792	$CoLi_{0.5}O_2$	10.46	$\eta_{4I}=1; z_{2I,1}=1; z_{2I,2}=0; z_{2I,3}=1$
icsd_020953	Co_4GaY_4	12.62	$\eta_{4I}=1; z_{2I,1}=0; z_{2I,2}=0; z_{2I,3}=1$
icsd_084195	Se_4V_3	12.62	$\eta_{4I}=1; z_{2I,1}=0; z_{2I,2}=0; z_{2I,3}=1$
icsd_201787	Mo_2S_4V	12.62	$\eta_{4I}=1; z_{2I,1}=0; z_{2I,2}=0; z_{2I,3}=1$
icsd_624816	$CoRh_2Se_4$	12.62	$\eta_{4I}=3; z_{2I,1}=1; z_{2I,2}=1; z_{2I,3}=1$
icsd_632972	$FeNi_2Se_4$	12.62	$\eta_{4I}=1; z_{2I,1}=0; z_{2I,2}=0; z_{2I,3}=1$

TABLE S63. ICSD numbers, chemical formulas, magnetic space groups (MSGs), and symmetry indicators for magnetic Smith-index semimetals (SISM).

ICSD	Formula	MSG	Symmetry indicators
icsd_646388	NiS_4Ti_2	12.62	$\eta_{4I}=1; z_{2I,1}=1; z_{2I,2}=1; z_{2I,3}=0$
icsd_646544	$NiSe_4Ti_2$	12.62	$\eta_{4I}=1; z_{2I,1}=1; z_{2I,2}=1; z_{2I,3}=0$
icsd_095948	NiO_3Tl	14.79	$\eta_{4I}=3; z_{2I,1}=1$
icsd_239671	Ca_2CrO_6Os	14.79	$\eta_{4I}=1; z_{2I,1}=1$
icsd_031343	$Li_{0.33}Se_2Ti$	12.62	$\eta_{4I}=1; z_{2I,1}=0; z_{2I,2}=0; z_{2I,3}=1$
icsd_076020	O_2PTi_3	164.89	$\eta_{4I}=3; z_{2I,3}=1; z_{3R}=1$
icsd_025561	STi	12.62	$\eta_{4I}=1; z_{2I,1}=0; z_{2I,2}=0; z_{2I,3}=0$
icsd_189226	Co_3SiTi_2	11.54	$\eta_{4I}=1; z_{2I,1}=0; z_{2I,3}=0$
icsd_190988	CoMnS	119.319	$\delta_{2S}=1; z_2=0; z_{4S}=2$
icsd_190989	CoMnSe	119.319	$\delta_{2S}=1; z_2=0; z_{4S}=2$
icsd_052971	Co_2GeMn	166.101	$\eta_{4I}=3; z_{2I,1}=0; z_{2I,2}=0; z_{2I,3}=0$
icsd_053312	Cu_2MnSb	166.101	$\eta_{4I}=1; z_{2I,1}=0; z_{2I,2}=0; z_{2I,3}=0$
icsd_053687	$GeMnNi_2$	166.101	$\eta_{4I}=3; z_{2I,1}=0; z_{2I,2}=0; z_{2I,3}=0$
icsd_076080	$MnNi_2Sb$	166.101	$\eta_{4I}=3; z_{2I,1}=0; z_{2I,2}=0; z_{2I,3}=0$
icsd_103813	$GaMn_2V$	166.101	$\eta_{4I}=1; z_{2I,1}=0; z_{2I,2}=0; z_{2I,3}=0$
icsd_103892	$GaNi_2V$	166.101	$\eta_{4I}=3; z_{2I,1}=0; z_{2I,2}=0; z_{2I,3}=0$
icsd_188333	Mn_3Sn	166.101	$\eta_{4I}=1; z_{2I,1}=0; z_{2I,2}=0; z_{2I,3}=0$

D. Table of Magnetic Enforced Semimetals with Fermi Degeneracy

Enforced semimetals with Fermi degeneracy (ESFD) are topological semimetals whose band degeneracies are symmetry-enforced at high-symmetry points of the Brillouin zone. In this subsection, we summarize all magnetic ESFD in a series of tables. These tables list the ICSD numbers, chemical formulas, and MSGs.

TABLE S64. ICSD numbers, chemical formulas, and magnetic space groups (MSGs) for magnetic enforced semimetals with Fermi degeneracy (ESFD).

ICSD	Formula	MSG	ICSD	Formula	MSG
icsd_671146	H_3MgNi_2	12.61	icsd_613152	B_4Co_4Lu	137.51
icsd_074165	$CaCu_2O_7Sr_2Tl$	123.347	icsd_613410	B_4Co_4Y	137.51
icsd_252344	As_4CaFe_4Rb	123.344	icsd_023653	B_2Co_2Y	71.535
icsd_057651	$AlCr_2$	71.535	icsd_052999	Co_2LaSi_2	71.535
icsd_074877	As_2CsFe_2	139.536	icsd_053088	Co_2Si_2Y	71.535
icsd_095837	$CsMn_2P_2$	71.535	icsd_053491	Fe_2LaSi_2	71.535
icsd_100438	Co_2S_2Tl	139.536	icsd_053556	Fe_2Si_2Y	71.535
icsd_167329	As_2Fe_2Rb	71.535	icsd_080506	Ge_2LaMn_2	69.523
icsd_189036	As_2Fe_2K	71.535	icsd_081748	Co_2Ge_2Y	69.523
icsd_424686	KNi_2Se_2	139.536	icsd_087581	Co_2LaP_2	69.523
icsd_641273	KNi_2S_2	139.536	icsd_610073	As_2Co_2La	69.523
icsd_646396	Ni_2S_2Tl	139.536	icsd_623465	Co_2Ge_2Lu	69.523
icsd_646550	Ni_2Se_2Tl	139.536	icsd_624957	Co_2ScSi_2	71.535
icsd_658698	$CsFe_2Sb_2$	69.523	icsd_632411	Fe_2LaP_2	139.536
icsd_042529	BMn_2	140.546	icsd_429102	$As_5La_4Mn_2$	12.61
icsd_614745	B_2Mn	140.546	icsd_086369	MnScSi	189.223
icsd_067400	Cr_2N	12.61	icsd_099080	$Ga_2Lu_3Mn_3Si$	189.223
icsd_167802	NV_2	12.6	icsd_643653	MnSiTa	189.224
icsd_024176	$Ni_3Pb_2S_2$	166.97	icsd_023550	B_2Co_3Hf	191.238
icsd_041381	Fe_6Ge_4Li	166.1	icsd_044191	B_2Co_3Zr	191.238
icsd_157323	Fe_2InO_4	166.1	icsd_079972	Ge_6LuMn_6	65.483
icsd_041459	Co_6Ge_6Li	191.241	icsd_623474	Co_6Ge_6Lu	191.241
icsd_057518	Al_9BaFe_2	191.236	icsd_623581	Co_6Ge_6Sc	191.241
icsd_658018	Cr_6Ge_6Y	191.239	icsd_624660	CoP_2W	194.268
icsd_187992	$AlCo_3$	194.269	icsd_652343	$SiTa_2V_3$	194.271
icsd_043860	$CAlMn_3$	166.97	icsd_102433	Co_2GaHf	71.535
icsd_044351	$CGeMn_3$	166.97	icsd_102646	Co_2ScSn	71.535
icsd_077153	CMn_3Sn	166.97	icsd_065295	$Cs_4Cu_3F_{10}$	2.6
icsd_015904	Cr_3O	167.106	icsd_079695	$H_2As_2CuFe_2O_{10}$	2.6
icsd_016835	Cr_3Si	167.106	icsd_186046	Fe_4Ge_2Lu	58.396
icsd_053127	Cr_3Ge	167.106	icsd_615659	B_4V_3	71.535
icsd_104020	GaV_3	167.106	icsd_107586	$BiNi_9S_8Te$	47.251
icsd_025324	Co_2GeLi	166.1	icsd_169733	Co_2GaNi	71.535
icsd_016894	Co_2N	58.399	icsd_069692	Co_6LiP_4	187.211
icsd_055578	$Co_2In_5Zr_4$	10.44	icsd_094412	Co_6MgP_4	187.211
icsd_171433	$BaCo_2O_5Y$	47.251	icsd_290889	FePTi	189.224
icsd_195900	$AsLaNNi_2$	63.46	icsd_410967	$In_3Rh_2Ti_3$	189.223
icsd_083690	$BaMn_2O_5Y$	123.347	icsd_610509	AsFeNi	189.223
icsd_096951	$KO_5S_2Ti_2Y_2$	123.347	icsd_610530	AsFeTi	189.223
icsd_153495	$BaCo_2LaO_6$	65.483	icsd_632938	FeNiP	189.223
icsd_171432	$BaCo_2O_5Y$	123.347	icsd_057808	$AlFe_2Ni$	166.1
icsd_186045	Fe_4Ge_2Lu	58.395	icsd_103460	Fe_2GaNi	139.536
icsd_633444	Fe_4ScSi_2	136.495			

E. Table of Magnetic Enforced Semimetals

Enforced semimetals (ESs) are topological semimetals whose band degeneracies are symmetry-enforced along high-symmetry lines or planes in the Brillouin zone. In this subsection, we summarize all magnetic ESs in a series of tables. These tables list the ICSD numbers, chemical formulas, and MSG.

TABLE S65. ICSD numbers, chemical formulas, and magnetic space groups (MSGs) for magnetic enforced semimetals (ES).

ICSD	Formula	MSG	ICSD	Formula	MSG
icsd_181037	$Cr_{0.5}Ga_{0.5}P$	115.287	icsd_622529	Co_2CsS_2	69.524
icsd_050819	$MnRbSe_2$	119.319	icsd_622533	Co_2CsSe_2	69.524
icsd_087983	$KMnTe_2$	119.319	icsd_623956	Co_2KS_2	71.536
icsd_087984	$MnRbTe_2$	119.319	icsd_624798	Co_2RbSe_2	69.524
icsd_096699	CuO_2	12.58	icsd_633338	Fe_2S_2Tl	139.537
icsd_160557	Ca_2CoO_3	12.58	icsd_024161	FeSSb	14.75
icsd_016809	BFe_2	23.51	icsd_024570	$FeSn_2$	69.524
icsd_005257	$FeSi_2$	123.345	icsd_024571	$MnSn_2$	72.544
icsd_028837	OPd	47.252	icsd_042519	$FeGe_2$	140.547
icsd_028918	$BaFeO_3$	123.345	icsd_042530	BFe_2	69.524
icsd_044806	LaSb	123.345	icsd_086940	O_3RuSr	140.547
icsd_053543	FeSe	47.252	icsd_102672	$CoSn_2$	69.524
icsd_057969	AlMn	123.345	icsd_186636	$FeSb_2$	69.524
icsd_098427	AsLa	123.345	icsd_425309	BFe	70.529
icsd_103989	GaTi	65.486	icsd_613476	BCr	74.559
icsd_173434	FeO_2Sr	65.486	icsd_050817	$LiMnSe_2$	8.32
icsd_173438	$CaFeO_2$	65.486	icsd_050818	$MnNaSe_2$	8.32
icsd_187255	MgNi	123.345	icsd_110774	$MnNaTe_2$	8.32
icsd_237789	$BaOSb_2Ti_2$	47.252	icsd_069332	$C_3D_3LaO_6$	160.67
icsd_430063	$BaBi_2OTi_2$	47.252	icsd_187684	NiO_3Pb	161.71
icsd_430299	$CsOS_2V_2$	47.252	icsd_200709	LiS_2Ti	12.58
icsd_634628	GaMn	47.252	icsd_609482	Al_3Tc_2	164.89
icsd_104026	Ga_5V_2	55.358	icsd_625401	$CoTe_2$	12.58
icsd_249632	Ga_5Mn_2	65.486	icsd_644993	NaS_2V	12.58
icsd_401730	In_5Ti_2	127.391	icsd_005436	$Co_3In_2S_2$	12.58
icsd_615683	B_4W	127.393	icsd_005437	Co_3InS_2Sn	166.101
icsd_015289	$BaNiS_2$	59.407	icsd_023354	BrLa	12.58
icsd_042327	FeLiP	59.407	icsd_024410	ClLa	12.58
icsd_042750	AlGeMn	129.417	icsd_026608	$LiNiO_2$	12.58
icsd_107932	AsCoLi	129.417	icsd_100217	$Ni_3S_2Sn_2$	12.58
icsd_162808	AsFFeSr	59.407	icsd_189825	LiS_2Ti	12.58
icsd_162902	CoSe	59.41	icsd_416314	$Co_{1.5}SSn$	12.58
icsd_237581	$ClNiO_3Sr_2$	67.506	icsd_016675	F_3Pd	15.85
icsd_418853	CoGeMg	129.417	icsd_080772	MnN_3Sr_3	176.143
icsd_428148	CaCoSi	129.416	icsd_650662	Ru_3Si_2Y	176.143
icsd_187715	NOs	131.441	icsd_077371	Si_2V	180.171
icsd_009423	CrO_2	136.501	icsd_638088	Ge_2V	180.169
icsd_035382	F_6LiV_2	136.501	icsd_096025	Si_2V	181.177
icsd_154021	O_2Re	136.499	icsd_042542	CFe_3	182.183
icsd_026560	MnO_4Sr_2	71.536	icsd_161882	$Al_{0.75}NZr_{0.25}$	186.207
icsd_055710	$CuI_2O_2Sr_2$	71.536	icsd_168896	BTc	186.207
icsd_067362	Co_2Se_2Tl	69.524	icsd_649860	Pt_3Y_7	36.175
icsd_067370	Co_2KSe_2	71.536	icsd_104487	IrLi	187.213
icsd_069849	FeO_4Sr_2	71.536	icsd_169398	CLa	187.213
icsd_106932	MnN	69.524	icsd_182014	NTc	187.213
icsd_167013	$As_2F_2OSr_2Ti_2$	71.536	icsd_185568	NZr	187.213
icsd_168287	Hf_2Tl	71.536	icsd_185572	NRu	38.189
icsd_186572	Fe_2KS_2	69.524	icsd_290430	N_2Ta	187.213
icsd_186573	Fe_2KSe_2	71.536	icsd_290439	N_2Os	187.213
icsd_186574	Fe_2KTe_2	71.536	icsd_073339	I_3LiSc	188.219
icsd_245748	Cl_6NbRb_2	69.524	icsd_027140	$Al_8FeMg_3Si_6$	189.225
icsd_246483	CoO_4Sr_2	71.536	icsd_096905	$Al_9FeMg_3Si_5$	189.225
icsd_420975	$BaCo_2Ge_2$	139.537	icsd_030331	B_2V	65.486
icsd_425467	$CaFe_2Si_2$	71.536	icsd_030416	B_2Cr	65.486
icsd_610297	As_2CsRu_2	139.537	icsd_043664	B_2Mn	191.24

TABLE S66. ICSD numbers, chemical formulas, and magnetic space groups (MSGs) for magnetic enforced semimetals (ES).

ICSD	Formula	MSG	ICSD	Formula	MSG
icsd_044581	B_2Ru_3Y	65.486	icsd_169410	ScSn	119.319
icsd_103634	FeSn	191.24	icsd_169766	CrTe	44.231
icsd_181506	S_2Ti	191.24	icsd_183160	CY	160.67
icsd_182350	CN_3Ta_2	65.486	icsd_183166	CMo	119.319
icsd_182352	N_3OTa_2	65.486	icsd_183198	CdN	44.231
icsd_240144	Mn_6Sn_6Y	65.486	icsd_184925	AsMn	44.231
icsd_260251	Co_2In_9K	191.24	icsd_191171	MnSn	119.319
icsd_415256	Co_6Ge_6Mg	191.241	icsd_191788	MnP	119.319
icsd_613892	B_2Fe	191.24	icsd_025596	F_3Nb	123.345
icsd_109145	I_3Nb	193.26	icsd_029096	$BaFeO_3$	123.345
icsd_009497	AsMn	63.463	icsd_042929	$InNTi_3$	65.486
icsd_010486	$BaSe_3V$	194.27	icsd_042930	CTi_3Tl	65.486
icsd_015520	BaO_3Rh	194.27	icsd_042931	NTi_3Tl	123.345
icsd_015908	$InSc_3$	194.27	icsd_043417	OsSi	166.101
icsd_018130	Se_2Ta	63.463	icsd_043799	$BaMoO_3$	123.345
icsd_020009	PoTi	194.27	icsd_043847	$CAlCo_3$	123.345
icsd_023405	Fe_3Ge	194.27	icsd_044385	RhSi	123.345
icsd_024569	Fe_3Sn	194.27	icsd_051948	InLa	166.101
icsd_035029	$BaCrO_3$	63.464	icsd_051950	$InLa_3$	166.101
icsd_036620	$D_{0.9}Br_2La$	194.266	icsd_053125	Cr_3GaN	166.97
icsd_052503	TeTi	194.27	icsd_053461	Fe_3Ge	166.101
icsd_053090	CoTe	194.27	icsd_055601	AlFe	166.101
icsd_053215	CrSe	194.27	icsd_057596	AlCo	123.345
icsd_053230	CrTe	194.27	icsd_057932	$AlLa_3$	123.345
icsd_053970	MnSb	194.27	icsd_058037	AlNi	123.345
icsd_058805	BiMn	194.27	icsd_058038	$AlNi_3$	123.345
icsd_104978	Mn_3Sn	63.464	icsd_058107	AlOs	65.486
icsd_105427	NiTl	194.27	icsd_058146	AlRe	166.101
icsd_106098	SnV_3	194.268	icsd_058155	AlRu	123.345
icsd_106184	$TiZn_2$	63.463	icsd_058693	BeCo	65.486
icsd_107934	AsCr	194.27	icsd_058700	BeCu	65.486
icsd_108535	HMn	63.463	icsd_058734	BeRh	65.486
icsd_150620	FeSn	194.27	icsd_059438	$InNi_3$	166.101
icsd_151196	$InNi_3$	63.463	icsd_059523	$InSc_3$	123.345
icsd_154257	Br_3RbTi	63.457	icsd_076062	Mn_3NSn	166.101
icsd_191081	HCr	63.457	icsd_076790	CCo_3Mg	123.345
icsd_191785	MnP	63.464	icsd_077142	CoO_3Sr	65.486
icsd_603210	$AlLa_3$	63.463	icsd_077152	$CMgNi_3$	123.345
icsd_603351	$GaMn_3$	63.463	icsd_088982	O_3SrV	123.345
icsd_625031	Co_3Si	63.464	icsd_091062	FeO_3Sr	123.345
icsd_631740	Fe_3Ga	63.463	icsd_099085	$DSnTi_3$	123.345
icsd_640342	$InRu_3$	63.463	icsd_103451	Fe_3Ga	65.486
icsd_640656	$InTi_3$	194.266	icsd_103638	Fe_3Sn	65.486
icsd_652041	SeTi	194.27	icsd_103765	$GaLa_3$	123.345
icsd_670095	$AuNiO_2$	194.27	icsd_103856	$GaNi_3$	65.486
icsd_670857	B_4Fe	63.464	icsd_104658	LaMg	123.345
icsd_052963	CoGe	146.1	icsd_104722	La_3Sn	123.345
icsd_187195	GeMn	146.1	icsd_104730	LaTl	123.345
icsd_616878	BiNiSe	19.27	icsd_104732	La_3Tl	166.101
icsd_652380	SiTc	146.1	icsd_106087	$SnTi_3$	123.345
icsd_063230	BaS_3V	20.34	icsd_108129	CCo_3Sn	123.345
icsd_028647	$CdKN_3O_6$	47.252	icsd_108903	CrO_3Sr	123.345
icsd_028648	CdN_3O_6Rb	47.252	icsd_155928	CoSi	123.345
icsd_028649	$CdCsN_3O_6$	47.252	icsd_159440	MoN	123.345
icsd_028650	CdN_3O_6Tl	47.252	icsd_167812	Al_3V	123.345
icsd_042539	$CoSe_2$	61.436	icsd_167814	Al_3Ti	123.345
icsd_043715	CoS_2	61.436	icsd_183416	NTi	65.486
icsd_185888	CrO_2	61.436	icsd_183420	HfN	123.345
icsd_251565	O_2Rh	148.17	icsd_183951	LaS	123.345
icsd_251567	IrO_2	61.436	icsd_183952	LaSe	123.345
icsd_625403	$CoTe_2$	61.436	icsd_183953	LaTe	123.345
icsd_608469	$Al_{0.6}Mn_{0.4}$	92.115	icsd_186891	CdN	166.101
icsd_635637	Ga_2V_3	155.45	icsd_187483	O_3RhSr	123.345
icsd_181035	$Cr_{0.25}Ga_{0.75}P$	111.255	icsd_187637	O_3PbV	123.345
icsd_181036	$Cr_{0.75}Ga_{0.25}P$	160.67	icsd_187710	NTc	65.486
icsd_079936	CoN	119.319	icsd_187962	$AlCo_3$	65.486
icsd_159438	MoN	119.319	icsd_188415	MnO_3Sr	123.345
icsd_161755	NNi	119.319	icsd_191170	MnSn	123.345
icsd_167877	NW	119.319	icsd_191174	MnSb	123.345
icsd_169408	ScSi	44.231	icsd_191203	BaO_3V	123.345

TABLE S67. ICSD numbers, chemical formulas, and magnetic space groups (MSGs) for magnetic enforced semimetals (ES).

ICSD	Formula	MSG	ICSD	Formula	MSG
icsd_236825	CrN	123.345	icsd_623472	$CoGe_2Lu_2$	12.58
icsd_236831	CoN	123.345	icsd_623661	$Co_2Ge_4Y_3$	12.58
icsd_247066	Co_3InN	65.486	icsd_645402	Nb_2Se_4V	12.58
icsd_247648	AsLu	123.345	icsd_150696	Ca_2FeO_6Re	14.75
icsd_608581	AlMo	123.345	icsd_150258	$LaMnO_3$	15.85
icsd_022412	SiV_3	167.106	icsd_164176	$BaFe_2O_5Y$	47.252
icsd_102767	Cr_3Ga	167.105	icsd_670101	$AgCuO_2$	47.252
icsd_106108	$SnZr_3$	131.441	icsd_071520	$FeNbTe_2$	53.328
icsd_187147	H_3Fe	66.496	icsd_083907	$CrLaSb_3$	57.383
icsd_638098	Ge_3V	131.441	icsd_043204	FePZr	62.441
icsd_077714	OZr_2	134.477	icsd_049727	CoNbP	62.446
icsd_022321	NV	71.536	icsd_053716	GeMnZr	62.449
icsd_028681	OV	139.537	icsd_083987	LuMnSi	62.444
icsd_061323	CuO	71.536	icsd_191794	NiO_3Y	62.446
icsd_077650	OPd	139.537	icsd_191796	$LuNiO_3$	62.446
icsd_109296	CrO	139.537	icsd_196498	CrPTa	62.448
icsd_167855	NRu	166.101	icsd_406953	AsCoHf	62.446
icsd_167863	NOs	139.537	icsd_601866	CoGeY	62.446
icsd_169573	NiS_2	139.537	icsd_623795	CoHfSi	62.447
icsd_169767	CrTe	71.536	icsd_624636	CoPTa	62.446
icsd_181773	CRh	139.537	icsd_624662	CoPW	62.447
icsd_183167	CTc	139.537	icsd_625050	CoSiTa	62.449
icsd_184375	FeN	166.101	icsd_626157	CrHfSi	62.449
icsd_184377	CoN	71.536	icsd_626850	CrSiZr	62.444
icsd_185983	CIr	139.537	icsd_632263	FeHfSi	62.445
icsd_186875	MoP	166.101	icsd_632794	FeNbP	62.441
icsd_191173	MnSb	166.101	icsd_645178	NbPV	62.444
icsd_236807	MnN	139.537	icsd_656389	HfPV	62.444
icsd_236813	NNi	71.536	icsd_670834	CFe_2Ta	62.448
icsd_629532	D_2V	71.536	icsd_670835	$CFeTa_2$	62.449
icsd_670177	$FeSi_2$	139.537	icsd_670839	CFe_2W	62.448
icsd_027836	O_4Pt_3	166.101	icsd_670840	$CFeW_2$	62.449
icsd_041401	FeS_2	29.102	icsd_057645	Al_2CoY	63.463
icsd_186518	FeO_4Si	31.125	icsd_195898	$AsFe_2LaN$	63.465
icsd_015003	$FeSb_2$	34.156	icsd_200548	D_3CoZr	63.463
icsd_042726	FeS_2	34.159	icsd_632057	$FeGe_2Lu$	63.462
icsd_042727	$FeTe_2$	34.159	icsd_632162	$FeGe_2Y$	63.462
icsd_042728	$CoTe_2$	34.159	icsd_072872	CoO_4Re	65.486
icsd_025678	$CoTe_2$	58.397	icsd_016776	B_2CoW_2	71.536
icsd_025679	$FeTe_2$	58.397	icsd_040950	C_4CoSc_3	71.536
icsd_026756	FeS_2	58.397	icsd_072863	C_4FeSc_3	71.536
icsd_041724	As_2Fe	58.393	icsd_167658	H_2PdTi_2	71.536
icsd_041727	$FeSb_2$	58.393	icsd_614261	B_2FeW_2	71.536
icsd_042540	$CoSe_2$	58.397	icsd_614775	B_4Mn_2Ta	71.536
icsd_076120	$CoSb_2$	58.398	icsd_614782	B_4Mn_2W	71.536
icsd_194807	B_4Mn	58.393	icsd_416515	$FePd_2Se_2$	72.544
icsd_610034	As_2Co	58.398	icsd_173487	NiO_6ReSr_2	87.75
icsd_053146	CrN	59.407	icsd_042373	$CoGe_3La$	107.231
icsd_095957	Cu_2O_3Sr	59.409	icsd_059908	$FeGe_3La$	107.231
icsd_261526	ClLiNTi	59.41	icsd_181054	$Cd_{0.5}Cr_{0.5}Te$	25.59
icsd_152811	Fe_2N	60.417	icsd_047123	$LaNiO_2$	123.345
icsd_185887	CrO_2	60.424	icsd_051262	$Ca_2ClCuNb_3O_{10}$	47.252
icsd_009496	AsMn	62.448	icsd_074163	$Ba_2Cu_2O_7TlY$	65.486
icsd_030412	MnP	62.445	icsd_150261	$CoIn_5La$	47.252
icsd_030449	BFe	62.447	icsd_150703	$BaLaMn_2O_6$	47.252
icsd_043249	CoP	62.448	icsd_160691	CCr_2LaSi_2	65.486
icsd_076241	MnTe	62.449	icsd_246455	$Ba_{0.5}La_{0.5}MnO_3$	47.252
icsd_092330	$CaFeO_3$	62.446	icsd_623081	$CoGa_4Hf$	65.486
icsd_093507	NiO_3Tl	62.446	icsd_623111	$CoGa_8Lu_2$	65.486
icsd_670820	CAl_2Fe	62.447	icsd_623236	$CoGa_5Y$	123.345
icsd_670821	$CAlFe_2$	62.449	icsd_623237	$CoGa_8Y_2$	123.345
icsd_164774	CaO_3Rh	63.464	icsd_623947	$CoIn_5Y$	47.252
icsd_187136	AsFeNa	63.462	icsd_623948	$CoIn_8Y_2$	47.252
icsd_015927	MgO_3V	65.485	icsd_009967	$CoNb_4P$	124.353
icsd_020083	AlB_2Cr_2	65.486	icsd_043233	$CoNb_4Si$	124.353
icsd_020322	AlB_2Fe_2	65.485	icsd_053511	$FeNb_4Si$	66.496
icsd_025518	AlB_2Mn_2	65.486	icsd_086378	$FePTa_4$	124.353
icsd_645398	Nb_2Se_4V	8.32	icsd_623784	$CoHf_4P$	124.357
icsd_002371	$CoSi_2Zr_2$	12.58	icsd_624637	$CoPTa_4$	124.353
icsd_041746	$CoSc_2Si_2$	12.58	icsd_624677	$CoPZr_4$	124.353

TABLE S68. ICSD numbers, chemical formulas, and magnetic space groups (MSGs) for magnetic enforced semimetals (ES).

ICSD	Formula	MSG	ICSD	Formula	MSG
icsd_632255	$FeHf_4P$	66.496	icsd_636559	GeHfMn	38.189
icsd_632795	$FeNb_4P$	66.496	icsd_637098	GeMnTa	189.225
icsd_043016	B_2FeW_2	127.387	icsd_015995	Mn_2O_3Ta	65.486
icsd_613529	B_2CrNb_2	65.486	icsd_044171	B_2Co_3Lu	65.486
icsd_613557	B_2CrTa_2	65.486	icsd_044179	B_2Co_3Sc	191.238
icsd_080007	GeLaMn	59.407	icsd_044439	B_2LuRu_3	65.486
icsd_080203	CoLaOP	67.506	icsd_054273	Mn_6ScSn_6	65.486
icsd_085904	GeTiY	59.41	icsd_054928	Mn_6Sn_6Zr	65.486
icsd_088113	SiTiY	67.506	icsd_054930	$HfMn_6Sn_6$	65.486
icsd_088208	LuSiTi	59.41	icsd_057416	$LuMn_6Sn_6$	65.486
icsd_107617	GeLaTi	129.417	icsd_089433	Ge_6Mn_6Zr	65.486
icsd_162724	FeLaOP	59.407	icsd_186421	N_3Ta_2Ti	65.486
icsd_163496	AsFeLaO	59.407	icsd_104003	$Ga_3Ti_2Zr_3$	63.464
icsd_168586	$Fe_2O_6P_2Sc_2Sr_4$	59.407	icsd_168592	$La_6Mn_2S_{10}$	193.26
icsd_180528	$As_2Fe_2O_6Sc_2Sr_4$	59.407	icsd_604200	$NiPb_3Zr_5$	63.463
icsd_420654	$AsBa_2FeO_3Sc$	59.407	icsd_624928	$CoSb_3Zr_5$	63.464
icsd_617820	C_2FeSc	59.41	icsd_646460	$NiSb_3Zr_5$	63.464
icsd_624599	CoPPd	67.506	icsd_659152	$CrLa_5Pb_3$	193.26
icsd_636594	GeHfV	59.407	icsd_659153	La_5MnPb_3	63.464
icsd_638931	HfSiV	59.407	icsd_659154	$FeLa_5Pb_3$	193.26
icsd_061684	CCoY	47.252	icsd_659155	$CoLa_5Pb_3$	63.464
icsd_061691	CCoLu	47.252	icsd_009966	Co_3Sc_2Si	194.27
icsd_068525	Fe_4P_2Sc	58.398	icsd_053483	Fe_3GeZr_2	63.463
icsd_087172	Fe_4Si_2Zr	58.398	icsd_053558	Fe_3SiZr_2	63.464
icsd_130032	Cu_2Hf_2In	136.501	icsd_057617	Al_3CoLu_2	194.27
icsd_130034	Cu_2InZr_2	136.501	icsd_076678	NiPZr	63.463
icsd_189495	Ni_4P_2Y	136.501	icsd_103807	GaMnPt	194.27
icsd_611100	As_2Ni_4Y	65.486	icsd_409622	Fe_2ILa_2	63.464
icsd_633122	Fe_4P_2Zr	58.398	icsd_625123	$Co_{1.5}Si_{0.5}W$	63.465
icsd_053715	Ge_2Mn_2Y	71.536	icsd_670980	Nb_2Ni_3Si	194.27
icsd_082937	Mn_2Si_2Y	71.536	icsd_626558	CrPtSb	146.1
icsd_088211	GeHfV	71.536	icsd_186187	$Cr_{0.25}SZn_{0.75}$	111.255
icsd_090197	$LuRu_2Si_2$	69.524	icsd_186188	$Cr_{0.25}SeZn_{0.75}$	111.255
icsd_107040	Ge_2LuMn_2	71.536	icsd_076099	MnPdSb	44.231
icsd_191366	$FeHfO_6Sr_2$	69.524	icsd_090397	FeSbZn	44.231
icsd_604549	B_2Fe_2Lu	139.537	icsd_107122	NbRhSb	44.231
icsd_614264	B_2Fe_2Y	139.537	icsd_108294	CoHfSb	44.231
icsd_632475	Fe_2LuSi_2	71.536	icsd_108482	GaMnPt	119.319
icsd_605616	$AgNiSe_2$	8.32	icsd_190995	$CMnSc_2$	44.231
icsd_043278	$AgFeTe_2$	164.89	icsd_191001	$MnSc_2Sn$	44.231
icsd_073974	$AgNiO_2$	12.58	icsd_643329	$MnPd_2Sn$	139.537
icsd_193884	CrO_2Pd	12.58	icsd_671365	BiFePt	44.231
icsd_187087	$LaNiO_3$	15.85	icsd_671366	BiCoPt	44.231
icsd_053016	$CoNb_3S_6$	182.183	icsd_671367	BiNiPt	160.67
icsd_104913	$MnNb_3S_6$	182.183	icsd_028908	LaO_3Ti	123.345
icsd_632811	$FeNb_3Se_6$	20.31	icsd_028921	$CoLaO_3$	123.345
icsd_643023	$MnNb_3Se_6$	20.34	icsd_029119	$LaMnO_3$	65.486
icsd_645400	Nb_3Se_6V	20.34	icsd_033667	CdO_3Ti	123.345
icsd_651111	S_6Ta_3V	20.34	icsd_044430	$BLaRh_3$	123.345
icsd_020298	BFeNb	38.191	icsd_044864	Fe_3NPt	123.345
icsd_020876	$CoGa_2Zr_6$	189.225	icsd_053142	Cr_3NPt	166.101
icsd_024185	MnNbSi	38.191	icsd_053506	Fe_3NPd	123.345
icsd_041156	GeMnPd	189.225	icsd_058547	$AuNV_3$	166.97
icsd_042911	GeMnNb	38.191	icsd_076058	Mn_3NPt	166.101
icsd_061415	$Fe_2S_6Ta_9$	38.191	icsd_076763	CFe_3Zn	65.486
icsd_082530	$FeTe_2Zr_6$	38.191	icsd_076793	CCo_3Sc	123.345
icsd_083932	As_2CoZr_6	189.225	icsd_076797	CCo_3Zn	123.345
icsd_086364	FeGeSc	38.191	icsd_077154	CMn_3Zn	123.345
icsd_096249	$FeLu_6Sb_2$	38.191	icsd_051988	$InMnPd_2$	166.101
icsd_156949	$FeSb_2Zr_6$	38.191	icsd_053705	$GeMnPd_2$	139.537
icsd_402701	Al_2FeZr_6	38.191	icsd_057611	$AlCo_2Hf$	139.537
icsd_409925	GePdTi	38.189	icsd_057620	$AlCo_2Nb$	139.537
icsd_600156	GeMnSc	38.191	icsd_057634	$AlCo_2Ta$	139.537
icsd_610906	AsMnPd	38.191	icsd_058510	Au_2InTi	166.101
icsd_614205	BFeTa	38.191	icsd_076100	$MnPd_2Sb$	166.101
icsd_623801	CoHfSn	38.191	icsd_102441	Co_2GaNb	139.537
icsd_624869	$Co_2S_6Ta_9$	38.189	icsd_102451	Co_2GaTa	139.537
icsd_626517	CrPPd	189.225	icsd_102483	Co_2HfSn	139.537
icsd_631770	$FeGa_2Hf_6$	38.191	icsd_102554	Co_2NbSn	71.536
icsd_631856	$FeGa_2Zr_6$	38.191	icsd_102687	Co_2SnZr	139.537

TABLE S69. ICSD numbers, chemical formulas, and magnetic space groups (MSGs) for magnetic enforced semimetals (ES).

ICSD	Formula	MSG	ICSD	Formula	MSG
icsd_104945	$MnPd_2Sn$	139.537	icsd_020297	C_2Cr_2V	63.465
icsd_104980	Mn_2SnW	166.101	icsd_042629	CCr_3Ge	63.464
icsd_107955	$AsMnPd_2$	166.101	icsd_044188	B_3CoV	63.463
icsd_185119	$AlTiZr_2$	139.537	icsd_057009	C_2Cr_3	63.465
icsd_190994	$CMnSc_2$	71.536	icsd_189761	$SnTi_3$	63.459
icsd_190996	$MnSc_2Si$	139.537	icsd_291338	CCr_3P	63.459
icsd_190998	$GeMnSc_2$	139.537	icsd_291339	Cr_3NP	63.464
icsd_191000	$MnSc_2Sn$	71.536	icsd_609880	$CAsCr_3$	63.465
icsd_108896	CoO_3Sr	11.5	icsd_637012	GeMnNi	63.462
icsd_000453	$Ni_3S_2Sn_2$	12.58	icsd_043843	$Al_2B_2Ru_3$	65.486
icsd_026173	$CoMo_2S_4$	12.58	icsd_033704	B_4Cr_3	71.536
icsd_026976	Cr_3Se_4	12.58	icsd_044293	B_4Fe_2Mo	71.536
icsd_151873	$CrFe_2Se_4$	12.58	icsd_044446	B_4Mn_3	71.536
icsd_601347	Se_4Ti_3	12.58	icsd_613166	B_2CoMo_2	71.536
icsd_624884	CoS_4V_2	12.58	icsd_614748	B_4Mn_2Mo	71.536
icsd_626655	CrS_4V_2	12.58	icsd_066404	$BaCuFeLuO_5$	35.167
icsd_626873	Cr_3Te_4	12.58	icsd_167196	$FeSe_{0.875}$	25.59
icsd_633517	Fe_2Se_4V	12.58	icsd_023779	CrNNb	99.167
icsd_653087	Te_4TiV_2	12.58	icsd_025751	Cr_3GeN	18.19
icsd_041858	AsCoS	14.75	icsd_093241	$CuSb_3Ti_2$	115.285
icsd_602022	HFeTi	17.1	icsd_053505	FeNNi	65.486
icsd_081204	Ca_2FeO_6W	25.59	icsd_067711	$Ba_2Fe_3O_8Y$	47.252
icsd_629491	D_2FeTi	26.69	icsd_075730	$Ba_2Ca_2Cu_3HgO_8$	123.345
icsd_632217	H_2FeTi	26.69	icsd_076202	$MnRh_2Sb$	47.252
icsd_020082	AlB_4Cr_3	47.252	icsd_107862	$AlNi_3$	65.486
icsd_190616	Co_2NbSn	51.295	icsd_157788	Co_2GaNi	65.486
icsd_194435	BNbRu	51.294	icsd_168837	$H_2Mg_{0.5}Ti_{0.5}$	127.397
icsd_263013	Fe_3O_4	51.295	icsd_186722	Fe_2GaMn	123.345
icsd_421074	$Ca_2Ge_2Ni_3$	51.295	icsd_187493	$GaMnNi_2$	65.486
icsd_429116	BRuTa	51.295	icsd_187494	$FeGaNi_2$	65.486
icsd_623100	Co_2GaLa	51.296	icsd_005431	B_2FeMo_2	127.387
icsd_670573	CFe_2	57.385	icsd_088317	B_2V_3	65.486
icsd_612536	B_2BaNi_2	58.398	icsd_613327	$B_2Co_5Ta_3$	65.486
icsd_080372	C_2CrSc	59.407	icsd_644412	Mo_3Si_2	65.486
icsd_646747	Ni_3Sn	59.411	icsd_016844	$AsFe_2$	59.41
icsd_002421	CoMoP	62.446	icsd_042325	Mn_2Sb	129.417
icsd_016483	CoMnP	62.448	icsd_042329	$AsMn_2$	129.417
icsd_016593	CFe_3	62.444	icsd_093237	AsFeMn	129.417
icsd_025726	Co_2P	62.447	icsd_165984	$AsFeO_3Sr_2V$	59.41
icsd_041149	MnRhSi	62.446	icsd_180529	$As_2Cr_2Fe_2O_6Sr_4$	59.407
icsd_043521	CCo_3	62.444	icsd_248374	CoMnSb	67.506
icsd_043686	PRu_2	62.447	icsd_420653	$AsCrFeO_3Sr_2$	59.407
icsd_044858	Co_2Si	62.449	icsd_200014	MoO_6Rh_2	136.501
icsd_053079	CoSiTi	62.445	icsd_094079	$FeMoO_6Sr_2$	139.537
icsd_055622	Mn_3Sn_2	62.441	icsd_153292	$GaMnNi_2$	139.537
icsd_076084	MnNiSi	62.448	icsd_246541	Ba_2FeMoO_6	139.537
icsd_077856	PV_2	62.445	icsd_617225	$BiTi_2$	71.536
icsd_105931	Rh_2Sn	62.447	icsd_025760	$AsCr_3N$	140.543
icsd_165247	CoSiV	62.449	icsd_025775	$CGeMn_3$	72.544
icsd_165250	CoFeSi	62.449	icsd_029132	F_3Fe	5.13
icsd_165256	CoNiSi	62.448	icsd_643223	Mn_2P	5.13
icsd_167128	$CCoFe_2$	62.447	icsd_151457	AlO_4V_2	12.58
icsd_181711	CCr_3	62.446	icsd_671321	CRu_2	166.101
icsd_187138	CFe_2	62.448	icsd_054657	CuSnTi	186.205
icsd_246547	IrMnSi	62.446	icsd_670856	B_4Fe	187.213
icsd_260757	BFe_3	62.446	icsd_042402	Fe_2P	38.191
icsd_603579	BCo_2Fe	62.447	icsd_043394	Mn_2P	38.191
icsd_610084	AsCoMn	62.444	icsd_043913	AsCrNi	189.225
icsd_622489	CoCrP	62.441	icsd_043919	AsCrRh	38.191
icsd_623417	Co_2Ge	62.449	icsd_044003	AsMnRh	189.225
icsd_624646	CoPTi	62.446	icsd_044004	AsMnRu	38.191
icsd_626440	CrNiP	62.448	icsd_056969	$AsCo_2$	38.191
icsd_633111	FePTi	62.449	icsd_098945	BSi_2Ti_6	38.189
icsd_633291	Fe_3S	62.448	icsd_102686	CoSnZr	38.191
icsd_670816	CTi_3	62.444	icsd_107550	Co_2P	38.189
icsd_670817	CV_3	62.45	icsd_167625	InLaNi	189.225
icsd_670829	$CFeMo_2$	62.449	icsd_189959	MoPRu	189.225
icsd_670831	$CFeNi_2$	62.446	icsd_600596	CrNiP	38.191
icsd_670838	$CFeV_2$	62.446	icsd_600852	MnNiP	189.225
icsd_670862	Rh_3Si	62.446	icsd_610094	AsCoNi	38.189

TABLE S70. ICSD numbers, chemical formulas, and magnetic space groups (MSGs) for magnetic enforced semimetals (ES).

ICSD	Formula	MSG	ICSD	Formula	MSG
icsd_610130	$AsCr_2$	189.225	icsd_670707	CoFeGeZr	44.231
icsd_610275	AsCrTi	189.225	icsd_044369	Mn_4N	123.345
icsd_610532	AsFeV	38.191	icsd_044659	$IrMn_3N$	65.486
icsd_610883	AsMnNi	38.191	icsd_044865	Fe_3NNi	166.101
icsd_610927	AsMnTi	189.225	icsd_053132	Cr_3IrN	166.101
icsd_623254	CoGaZr	38.191	icsd_053143	Cr_3NRh	166.101
icsd_643230	MnPRh	189.225	icsd_053502	Fe_4N	123.345
icsd_643671	MnSiTi	189.225	icsd_077369	$Fe_{11}Si_5$	123.345
icsd_036504	$BCaNi_4$	191.24	icsd_077394	CRu_3V	123.345
icsd_102458	Co_3Ga_2Y	65.486	icsd_153274	Fe_3NRh	166.101
icsd_160914	$H_{12}Fe_5La$	65.486	icsd_183372	$CuNNi_3$	65.486
icsd_601122	BFe_4Lu	65.486	icsd_052954	$CoFe_2Ge$	166.101
icsd_613036	BCo_3FeY	191.24	icsd_052958	Co_2FeSi	139.537
icsd_613133	BCo_4La	65.486	icsd_053002	Co_2MnSb	139.537
icsd_024359	Mn_5Si_3	63.463	icsd_053007	Co_2MnSi	139.537
icsd_042585	Fe_5Si_3	193.26	icsd_053080	Co_2SiTi	139.537
icsd_044386	Si_3Ti_5	193.26	icsd_053462	Fe_3Ge	71.536
icsd_103996	Ga_3Ti_5	193.26	icsd_053525	$FeRu_2Si$	166.101
icsd_103997	Ga_4Ti_5	193.26	icsd_053545	Fe_3Si	139.537
icsd_191489	BSi_3V_5	193.257	icsd_057600	$AlCo_2Cr$	139.537
icsd_609885	CAs_3V_5	63.464	icsd_057607	$AlCo_2Fe$	139.537
icsd_613552	BCr_5Si_3	63.464	icsd_057618	$AlCo_2Mn$	166.101
icsd_614407	BGe_3V_5	63.464	icsd_057654	$AlCrFe_2$	139.537
icsd_617535	CCr_5Si_3	193.26	icsd_057662	$AlCrNi_2$	139.537
icsd_637143	Ge_3Mo_5	193.26	icsd_057695	$AlCu_2Mn$	166.101
icsd_638048	Ge_3Ti_5	193.26	icsd_057793	$AlFe_3$	166.101
icsd_643689	$Mn_3Si_3V_2$	193.26	icsd_057806	$AlFe_2Mn$	71.536
icsd_644410	Mo_5Si_3	193.26	icsd_057827	$AlFe_2Ti$	166.101
icsd_041921	GeMnNi	194.27	icsd_057832	$AlFe_2V$	166.101
icsd_052020	$GeMn_2$	63.464	icsd_057986	$AlMnRh_2$	166.101
icsd_053006	CoMnSi	63.464	icsd_076700	Ni_2SbTi	139.537
icsd_053460	Fe_2Ge	191.24	icsd_102318	Co_2CrGa	139.537
icsd_102582	CoNiSn	194.27	icsd_102385	$CoFe_2Ga$	166.101
icsd_102673	Co_2Sn	194.27	icsd_102386	Co_2FeGa	139.537
icsd_104976	Mn_2Sn	63.463	icsd_102392	Co_2FeIn	139.537
icsd_108289	Co_2Ge	63.463	icsd_102438	Co_2GaMn	166.101
icsd_108590	MnNiSi	63.463	icsd_102453	Co_2GaTi	139.537
icsd_163332	Mn_2Sb	194.27	icsd_102456	Co_2GaV	166.101
icsd_181132	FeSbV	63.463	icsd_102682	Co_2SnTi	139.537
icsd_182095	B_4Mo	63.463	icsd_102684	Co_2SnV	166.101
icsd_623495	CoGeMn	63.464	icsd_102755	$CrFe_2Ga$	139.537
icsd_624067	Co_2Mg	63.464	icsd_102996	Cu_2InMn	166.101
icsd_044660	IrMnSb	160.67	icsd_103057	Cu_2MnSn	166.101
icsd_053071	CoSbV	160.67	icsd_103469	Fe_2GaTi	139.537
icsd_053537	FeSbTi	160.67	icsd_103473	Fe_2GaV	71.536
icsd_053539	FeSbV	119.319	icsd_103615	$FeRu_2Sn$	166.101
icsd_054255	MnNiSb	44.231	icsd_103641	Fe_2SnTi	166.101
icsd_104498	IrMnSn	160.67	icsd_103644	Fe_2SnV	166.101
icsd_106496	CoSnTi	44.231	icsd_105376	Ni_2SnV	139.537
icsd_107127	RuSbTi	119.319	icsd_105933	Rh_2SnV	166.101
icsd_108492	GaRhTi	160.67	icsd_108436	Fe_3Ga	139.537
icsd_161713	MnNiSi	44.231	icsd_151206	Cu_2FeSn	166.101
icsd_184948	Mn_2Sb	44.231	icsd_151207	$CoCu_2Sn$	71.536
icsd_185079	CoSnV	119.319	icsd_185966	$AlCo_2Ti$	139.537
icsd_185882	$AlTi_2Zn$	119.319	icsd_185999	$CrFe_2Sn$	71.536
icsd_189696	$AlTi_2$	119.319	icsd_186056	Fe_2InTi	166.101
icsd_189699	$GaTi_2$	119.319	icsd_186059	$AsFe_2Ti$	166.101
icsd_189705	$SiTi_2$	44.231	icsd_186060	Fe_2SbTi	71.536
icsd_189708	$GeTi_2$	160.67	icsd_186065	Fe_2GeMn	166.101
icsd_189711	$SnTi_2$	44.231	icsd_186721	Fe_2GaMn	166.101
icsd_190990	CoMnTe	119.319	icsd_188332	$GaMn_3$	166.101
icsd_191683	FeTeV	119.319	icsd_416260	Co_2CrIn	139.537
icsd_191685	CrFeTe	44.231	icsd_608800	$AlNi_3$	166.101
icsd_623808	Co_2HfSn	139.537	icsd_623481	$Co_{8.8}Ge_4Mn_{3.2}$	139.537
icsd_625319	Co_2SnZr	139.537	icsd_671340	$GeRu_2V$	166.101
icsd_670704	MnSiVZr	44.231	icsd_671341	Ru_2SbV	166.101
icsd_670706	CoFeSiZr	160.67			

F. Table of Linear Combinations of Elementary Band Representation

Linear combinations of elementary band representations (LCEBR) indicate phases that do not exhibit symmetry-protected topological features. In this subsection, we summarize all magnetic LCEBR in a series of tables. These tables list the ICSD numbers, chemical formulas, and MSGs.

TABLE S71. ICSD numbers, chemical formulas, and magnetic space groups (MSGs) for magnetic linear combinations of elementary band representation (LCEBR).

ICSD	Formula	MSG	ICSD	Formula	MSG
icsd_039351	MnO_6SbSr_2	107.231	icsd_182323	NaO_2V	12.58
icsd_001029	CoI_4Rb_2	11.53	icsd_250692	$C_2CoN_2S_2$	12.58
icsd_002232	CuI_2O_6	11.5	icsd_251654	CrI_3	12.62
icsd_036581	$HCuO_5STl$	11.5	icsd_260368	$H_4O_{10}V_4$	12.58
icsd_036582	$HCuO_5SeTl$	11.5	icsd_262639	Cl_3Tc	12.6
icsd_166586	F_5KNOOs	11.53	icsd_403035	Cl_4CrLi_2	12.62
icsd_166587	CsF_5NOOs	11.53	icsd_423461	Br_4W	12.6
icsd_170771	$MnNaO_4Rb_2$	11.54	icsd_602341	$NiPS_3$	12.61
icsd_187148	H_4Fe	11.53	icsd_611574	As_2V	12.6
icsd_246090	Ca_2MnO_6Sb	11.54	icsd_624616	$Co_2P_2S_6$	12.6
icsd_411140	Cl_7CsTi_2	11.52	icsd_626521	$CrPSe_3$	12.58
icsd_422751	$CuNa_2O_2$	11.53	icsd_646145	$NiPSe_3$	12.6
icsd_631817	$FeGa_2Se_4$	111.255	icsd_647926	$P_2Pd_2S_6$	12.61
icsd_246244	$CaFeO_2$	18.19	icsd_648076	$P_2S_6V_2$	12.61
icsd_102500	$CoIn_3$	34.158	icsd_657314	$Ni_2P_2S_6$	12.61
icsd_631756	$FeGa_3$	34.158	icsd_670347	$CaMnO_3$	12.62
icsd_150822	FeS_2Tl	119.319	icsd_108934	CrK_3O_4	42.221
icsd_633509	$FeSe_2Tl$	119.319	icsd_108935	K_3MnO_4	42.221
icsd_004073	CrI_2	12.58	icsd_172506	$GeMnTe_4Tl_2$	121.331
icsd_009485	$H_4CuF_2O_2$	12.62	icsd_172507	$MnSnTe_4Tl_2$	121.331
icsd_015596	$H_4Cl_2MnO_2$	12.58	icsd_608538	Al_2MnTe_4	42.221
icsd_015597	$H_4Cl_2FeO_2$	12.62	icsd_639984	In_2MnTe_4	42.221
icsd_016225	NiO_6Sr_2Te	12.62	icsd_659100	Ga_2MnSe_4	42.221
icsd_016252	$Fe_2P_2S_6$	12.61	icsd_004199	$CoKO_2$	24.55
icsd_016270	$MnNaO_2$	12.62	icsd_021072	F_4FeRb	47.252
icsd_017013	CoO	12.58	icsd_027689	CuF_3K	65.486
icsd_021055	Ba_2CuF_6	12.62	icsd_027690	CrF_3K	47.252
icsd_022079	Br_2Cu	12.62	icsd_043457	CuF_3Tl	65.486
icsd_022080	Cl_3Cr	12.62	icsd_069675	Cs_2F_5Mn	123.345
icsd_022082	$H_4Cl_2CoO_2$	12.58	icsd_075868	$CaCuO_2$	123.345
icsd_022084	$H_4Br_2MnO_2$	12.58	icsd_082218	F_5MnRb_2	123.345
icsd_022085	$H_4Br_2CoO_2$	12.58	icsd_109293	CuF_3Rb	65.486
icsd_023903	Br_2Cr	12.62	icsd_412972	Na_5NiO_2S	123.345
icsd_026108	Cl_3Mo	12.61	icsd_412978	$CoNa_5O_2S$	47.252
icsd_026609	$NaNiO_2$	12.58	icsd_021110	CuF_3K	55.358
icsd_026667	Cl_2Cu	12.62	icsd_085499	F_4FeRb	127.387
icsd_030011	FeS_2Tl	12.61	icsd_245749	Cl_6K_2Nb	58.398
icsd_031320	$C_2N_2NiS_2$	12.62	icsd_010454	Bi_2CaMn	59.407
icsd_042077	P_2V	12.61	icsd_015770	$CoKO_2$	129.417
icsd_043898	As_2Cr	12.6	icsd_026458	$LiMnP$	59.407
icsd_047223	IrK_4O_4	12.62	icsd_026459	$AsLiMn$	59.407
icsd_049021	$KLiMnO_2$	12.6	icsd_026460	$MnNaP$	59.407
icsd_060263	$D_4Cl_2CoO_2$	12.58	icsd_026462	$MnNaSb$	59.407
icsd_061391	$MnPS_3$	12.61	icsd_026889	$FeSe$	59.407
icsd_061392	$FePS_3$	12.61	icsd_040572	$AsCsMn$	59.407
icsd_072287	Cs_4IrO_4	12.62	icsd_041869	$CsMnSb$	59.407
icsd_072389	Ca_2FeN_2	12.61	icsd_041882	$KMnP$	59.407
icsd_075454	$As_2Ba_2Mn_2O$	12.61	icsd_041883	$AsKMn$	59.407
icsd_076548	$NaSe_2V$	12.62	icsd_042977	FeS	59.407
icsd_076670	NiO	12.62	icsd_044753	$FeTe$	59.407
icsd_096556	$CaClFeO_2$	12.6	icsd_050988	$ClKMoO_5P$	129.417
icsd_100354	$FeSe_2Tl$	12.6	icsd_050989	$ClMoO_5PRb$	129.417
icsd_160556	CoO_2	12.62	icsd_052758	$CaGeMn$	59.407
icsd_169194	CoO_6Pb_2Te	12.62	icsd_053707	$GeMnSr$	59.407
icsd_174134	$CuLi_2O_2$	12.62	icsd_059359	Li_2O_5SiV	129.417

TABLE S72. ICSD numbers, chemical formulas, and magnetic space groups (MSGs) for magnetic linear combinations of elementary band representation (LCEBR).

ICSD	Formula	MSG	ICSD	Formula	MSG
icsd_060736	BiMnNa	129.416	icsd_000406	$CaCo_2Ge_2$	71.535
icsd_066948	GeMgMn	59.407	icsd_000407	Co_2Ge_2Sr	71.535
icsd_066949	CaMnSi	59.407	icsd_001139	Cl_4MnRb_2	71.536
icsd_066950	CaMnSn	59.407	icsd_010463	$CaFe_2P_2$	69.523
icsd_066951	MnSnSr	59.407	icsd_010466	Co_2P_2Sr	69.523
icsd_082639	$BaCoS_2$	67.503	icsd_010467	Fe_2P_2Sr	139.536
icsd_086777	$GeLi_2O_5V$	129.417	icsd_010468	$BaFe_2P_2$	69.523
icsd_088460	$FFeO_3Sr_2$	67.503	icsd_015372	CuF_4K_2	69.524
icsd_089590	KMnSb	59.407	icsd_021069	K_2NiO_2	71.536
icsd_089594	MnPRb	59.407	icsd_032019	$BaMn_2Sb_2$	71.535
icsd_089596	AsMnRb	59.407	icsd_041571	Cl_4CrCs_2	71.536
icsd_089598	CsMnP	59.407	icsd_041794	As_2BaMn_2	71.535
icsd_090122	$ClCoO_3Sr_2$	67.506	icsd_053059	CoO	71.536
icsd_093508	$ClFeO_3Sr_2$	59.407	icsd_065259	Cs_2CuF_6	69.524
icsd_093509	$BrFeO_3Sr_2$	67.503	icsd_073209	Na_2NiO_2Rb	139.537
icsd_096557	Ca_2ClFeO_3	59.407	icsd_074889	$CoCsK_2O_2$	69.524
icsd_162899	CrSe	59.407	icsd_100025	Bi_2MnSr	71.535
icsd_162900	MnSe	59.407	icsd_163209	As_2Fe_2Sr	71.535
icsd_162903	NiSe	129.417	icsd_166016	As_2CaFe_2	71.535
icsd_163143	AsFeNa	59.407	icsd_167014	$F_2OSb_2Sr_2Ti_2$	71.536
icsd_189939	FMnPSr	59.407	icsd_183149	$Ba_2F_2Mn_2OSe_2$	71.536
icsd_189940	AsFMnSr	59.407	icsd_236760	O_4Sr_2Tc	71.536
icsd_189941	FMnSbSr	59.407	icsd_249687	$Ba_2F_2Fe_2OSe_2$	71.536
icsd_248364	BaFMnSb	59.407	icsd_249690	$F_2Fe_2OSe_2Sr_2$	71.536
icsd_248365	AsBaFMn	59.407	icsd_252590	$BaBi_2Mn_2$	71.535
icsd_290482	H_2Ti	129.419	icsd_405782	CoO_6Pb_2Te	71.536
icsd_426033	BaBiFMn	129.416	icsd_420974	$CaCo_2Si_2$	71.535
icsd_601586	BiKMn	129.416	icsd_425470	Co_2Si_2Sr	71.535
icsd_616575	BiCsMn	129.416	icsd_609848	As_2BaCo_2	71.535
icsd_616824	BiMnRb	129.416	icsd_609849	As_2BaCr_2	71.535
icsd_642150	LiMnSb	59.407	icsd_609899	As_2CaCo_2	71.535
icsd_010293	Cl_4Re	13.68	icsd_610122	As_2Co_2Sr	71.535
icsd_063686	ClF_6O_2Ru	13.68	icsd_610273	As_2Cr_2Sr	71.535
icsd_067168	Cl_7CsTi_2	13.67	icsd_004411	Cl_3MoO	14.77
icsd_186505	AsCaFFe	13.67	icsd_006024	CuF_2	14.75
icsd_186508	AsFFeSr	13.67	icsd_006044	F_6Li_2Rh	14.75
icsd_000393	MnO_2	65.486	icsd_010350	CrF_6Li_2	14.75
icsd_001504	O_2V	136.501	icsd_015590	Cl_3CuK	14.77
icsd_009165	F_2Mn	136.499	icsd_015889	O_2V	14.77
icsd_009166	F_2Fe	58.398	icsd_020453	AgF_2	14.79
icsd_009167	CoF_2	136.499	icsd_023722	MoO_2	14.77
icsd_009168	F_2Ni	65.486	icsd_026073	F_6Na_3Ni	14.79
icsd_015071	O_2Ru	136.499	icsd_027070	CrF_6Na_3	14.79
icsd_016763	F_2Pd	58.398	icsd_027347	F_6Na_3V	14.79
icsd_024794	Cr_2O_6Te	58.395	icsd_030410	CuO_6Sb_2	14.79
icsd_024795	Fe_2O_6Te	136.503	icsd_031827	CrF_2	14.75
icsd_032552	F_2V	58.398	icsd_034602	CuF_4Na_2	14.75
icsd_040344	FeO_6Sb_2	58.398	icsd_038384	HClCuO	14.77
icsd_072387	$CoLiN_2Sr_2$	136.501	icsd_042614	$CoSb_2$	14.75
icsd_074565	F_6Li_2Mo	58.398	icsd_054136	Br_3CrIn	14.78
icsd_076024	O_2Ta	136.501	icsd_061038	$K_2Mn_2O_3$	14.78
icsd_078778	CrF_4	136.502	icsd_062655	F_4LiMn	14.79
icsd_080802	NiO_6Sb_2	136.501	icsd_065510	I_6K_2Tc	14.75
icsd_084789	CuO_6Sb_2	58.398	icsd_065785	F_4V	14.79
icsd_095778	F_6Li_2Rh	58.398	icsd_066201	Cl_4CrNa_2	14.79
icsd_099714	MoO_2	136.499	icsd_066315	F_6MnNa_3	14.79
icsd_103447	$FeGa_3$	58.395	icsd_067250	CrF_4Na_2	14.79
icsd_108964	CoO_6Sb_2	65.486	icsd_069801	MnO_6Se_2	14.75
icsd_165210	F_6Li_2Ru	136.499	icsd_071455	F_4MnNa	14.79
icsd_168834	H_2Ti	58.398	icsd_074940	CoK_2O_2	14.77
icsd_201756	F_6Na_2Nb	65.486	icsd_079451	$CaIrO_6Sr_2$	14.75
icsd_262579	K_3NiO_2	58.398	icsd_083473	Ca_2FeO_6Sb	14.75
icsd_290252	F_6Li_2V	136.501	icsd_084791	Ca_3O_6Re	14.79
icsd_412062	Co_4In_{12}	58.398	icsd_084949	$HMnO_2$	14.77
icsd_418676	CrF_6Li_2	58.398	icsd_098698	HCuFO	14.75
icsd_424578	Cs_3NiO_2	58.398	icsd_153001	Ca_2CoO_6Te	14.75
icsd_424579	NiO_2Rb_3	58.398	icsd_153002	CoO_6Sr_2Te	14.79
icsd_074985	B_4Mn_4	67.503	icsd_165398	F_4Ru	14.75
icsd_000404	$BaGe_2Mn_2$	71.535	icsd_169193	CoO_6Pb_2Te	14.75
icsd_000405	$BaMn_2Sn_2$	139.536	icsd_173152	O_2Tc	14.77

TABLE S73. ICSD numbers, chemical formulas, and magnetic space groups (MSGs) for magnetic linear combinations of elementary band representation (LCEBR).

ICSD	Formula	MSG	ICSD	Formula	MSG
icsd_182568	CaO_6ReSr_2	14.75	icsd_042163	F_6HgRh	2.4
icsd_185809	AsFeS	14.77	icsd_054140	$MnPSe_3$	2.6
icsd_190486	Ca_2InO_6Os	14.75	icsd_054141	$FePSe_3$	2.6
icsd_190774	C_2NiO_4	14.75	icsd_056890	$Fe_2P_2Se_6$	2.6
icsd_193723	MnS_2	14.75	icsd_059175	KO_8S_2V	2.4
icsd_202451	CuO_3Te	14.77	icsd_059343	$BaCo_2O_8P_2$	148.19
icsd_202918	CoF_4Li	14.75	icsd_061217	$IrLi_8O_6$	2.4
icsd_238316	InO_6OsSr_2	14.79	icsd_063304	$FeI_{12}Y_7$	2.4
icsd_239557	Cl_3CuTl	14.77	icsd_063353	$AsNaNiO_4$	2.6
icsd_250364	Cl_4V	14.75	icsd_063544	$AsKNiO_4$	2.6
icsd_290251	F_6Li_2V	14.75	icsd_069591	$GeMnO_3$	2.6
icsd_290789	CrO_6SbSr_2	14.75	icsd_071020	$Cr_2Si_2Te_6$	148.17
icsd_290790	Ca_2CrO_6Sb	14.79	icsd_076421	Br_3Fe	2.4
icsd_411050	Cl_6Na_3Ti	14.75	icsd_079165	B_2MnO_6Sn	148.17
icsd_421461	AgF_4K_2	14.79	icsd_079268	$Cr_2Ge_2Te_6$	148.17
icsd_425100	B_4Mn	14.75	icsd_095776	F_6LiRh	148.17
icsd_425149	AgF_4Na_2	14.75	icsd_095777	F_6IrLi	148.17
icsd_610526	AsFeSe	14.77	icsd_165203	F_6LiRu	2.4
icsd_610529	AsFeTe	14.78	icsd_165206	F_6LiOs	148.17
icsd_633086	FePS	14.77	icsd_165208	F_6LiPt	2.4
icsd_633093	FePSe	14.77	icsd_165215	F_6KRh	2.4
icsd_633399	FeSbSe	14.77	icsd_169192	CoO_6Pb_2Te	148.17
icsd_633405	FeSbTe	14.77	icsd_174290	Ba_2BiIrO_6	2.4
icsd_008000	CuF_3K	140.545	icsd_182435	Mn_3O_6Te	2.6
icsd_042520	Sb_2Ti	140.543	icsd_240981	BaF_6Ir	148.17
icsd_052331	Sb_2V	72.541	icsd_251655	CrI_3	148.17
icsd_069656	CuF_3Rb	69.524	icsd_260062	$As_2BaCo_2O_8$	148.17
icsd_075412	F_3KMn	72.544	icsd_280167	$BaNi_2O_8P_2$	2.6
icsd_076127	BCr_2	72.541	icsd_408324	$Ca_2Li_6Mn_2N_6$	148.19
icsd_086811	$CrSb_2$	140.543	icsd_412874	$Li_6Mn_2N_6Sr_2$	148.19
icsd_169765	CrF_3K	72.544	icsd_418671	CrF_6Na	148.17
icsd_174206	MoO_3Sr	72.544	icsd_418672	CrF_6K	2.4
icsd_183452	O_3SrTc	140.541	icsd_418673	CrF_6Rb	2.4
icsd_248378	$BaIrO_3$	140.541	icsd_419467	$Ba_6N_6OOs_2$	2.4
icsd_031149	$Fe_2Li_2O_4$	70.53	icsd_424895	$BaFe_2O_8P_2$	2.6
icsd_043437	$FeLiO_2$	141.556	icsd_626809	$CrSiTe_3$	148.17
icsd_164158	LiO_2Ti	141.556	icsd_643237	$Mn_2P_2Se_6$	2.6
icsd_091527	$KNiO_9P_3$	146.1	icsd_670349	$CaMnO_3$	148.17
icsd_162264	$BiFeO_3$	1.1	icsd_060313	$IKNiO_6$	5.13
icsd_193740	$H_4As_3MnNS_6$	1.1	icsd_201056	$C_6Au_3CoKN_6$	5.13
icsd_073736	CsO_8S_2V	2.4	icsd_249724	$C_6Au_3KN_6Ni$	5.13
icsd_245667	$CsFeO_8S_2$	2.4	icsd_002790	CrP_4	15.87
icsd_250709	$BaCo_2O_8P_2$	147.15	icsd_006286	O_3V_2	15.88
icsd_002552	Cl_3MnNa	148.17	icsd_015557	$FeKS_2$	15.88
icsd_010343	$CaCrF_6$	2.4	icsd_038315	P_4V	15.87
icsd_010344	CrF_6Mg	2.4	icsd_040780	$FeKSe_2$	15.88
icsd_010347	CrF_6Hg	148.17	icsd_040781	$FeRbSe_2$	15.87
icsd_015108	F_6NiPb	2.4	icsd_202381	$FeRbS_2$	15.88
icsd_016316	Mo_3Se_4	148.19	icsd_075550	FeO_8RbSe_2	5.15
icsd_022081	Cl_3Cr	148.17	icsd_004266	FeO_4P	152.35
icsd_025010	F_6MnSn	2.4	icsd_025813	$BaCoO_2$	5.13
icsd_025011	F_6FeSn	2.4	icsd_010424	Ni_3S_2	5.15
icsd_025014	CoF_6Sn	148.17	icsd_110773	$LiMnTe_2$	8.34
icsd_025015	F_6NiSn	148.17	icsd_182698	$H_4Ni_3O_9Si_2$	157.55
icsd_025016	CuF_6Sn	148.17	icsd_022093	Cl_3Ru	9.39
icsd_027014	$As_2BaNi_2O_8$	2.6	icsd_001372	$HCrO_2$	160.67
icsd_027500	Cl_3Fe	148.19	icsd_001373	$DCrO_2$	160.67
icsd_027664	F_6KOs	148.17	icsd_024315	Se_2Ta	8.34
icsd_029203	MnO_3Sn	2.6	icsd_029312	NiS	160.65
icsd_033288	Cl_2CoO_8	148.17	icsd_036207	Fe_3O_7P	160.67
icsd_033289	Cl_2NiO_8	2.4	icsd_042596	NiSe	8.32
icsd_035145	$I_{12}Zr_6$	2.4	icsd_043410	S_2Ta	8.32
icsd_038236	Cl_3Ti	2.6	icsd_069571	$H_6F_3O_3V$	8.34
icsd_038237	Cl_3V	2.4	icsd_077990	RbS_2Ti	8.32
icsd_039242	Br_3Ti	2.4	icsd_088852	$AuCrS_2$	8.34
icsd_041539	$Cl_{12}Zr_6$	148.19	icsd_201396	CrS_2Tl	160.67
icsd_041540	$Br_{12}Zr_6$	148.19	icsd_401027	$Cl_8Na_2Ti_3$	8.32
icsd_042159	F_6MgRh	2.4	icsd_607619	Al_2FeS_4	8.32
icsd_042160	CaF_6Rh	2.4	icsd_608507	Al_2MnS_4	8.32
icsd_042161	F_6RhZn	2.4	icsd_626736	$CrSe_2Tl$	8.32

TABLE S74. ICSD numbers, chemical formulas, and magnetic space groups (MSGs) for magnetic linear combinations of elementary band representation (LCEBR).

ICSD	Formula	MSG	ICSD	Formula	MSG
icsd_634670	Ga_2MnS_4	8.34	icsd_246907	I_2V	12.58
icsd_639980	In_2MnSe_4	160.67	icsd_416038	$NaO_8Rb_3Ru_2$	12.6
icsd_641335	KS_2Ti	8.32	icsd_416040	$K_3NaO_8Ru_2$	12.6
icsd_644994	NaS_2V	8.32	icsd_425912	Cs_2F_6Tc	164.89
icsd_015299	$BiFeO_3$	9.39	icsd_425914	F_6K_2Tc	164.89
icsd_028917	$BaFeO_3$	9.39	icsd_425915	F_6Na_2Tc	164.89
icsd_200999	Li_2O_3Re	9.37	icsd_425918	F_6Rb_2Tc	164.89
icsd_246425	$BiCrO_3$	161.69	icsd_626052	$CrGa_2S_4$	164.89
icsd_252433	LiO_3Os	161.69	icsd_631804	$Fe_2Ga_2S_5$	12.6
icsd_001838	$BaFe_4O_8Sr$	12.58	icsd_632443	$FeLi_2S_2$	12.62
icsd_009484	$C_6D_3CoN_6$	162.77	icsd_634664	$Ga_2Mn_2S_5$	164.88
icsd_015174	$BaCaFe_4O_8$	12.58	icsd_000071	Fe_3Sn_2	166.101
icsd_029035	Cl_3Ti	12.6	icsd_001846	$Cl_8Mn_3Na_2$	166.101
icsd_080349	As_2NiO_6	12.58	icsd_004059	Cl_2Fe	12.62
icsd_080350	As_2CoO_6	162.77	icsd_006038	BaF_6Rh	166.101
icsd_187098	As_2O_6Pd	12.58	icsd_006152	$CoNaO_2$	12.58
icsd_201755	F_6Li_2Nb	12.62	icsd_009457	$Ba_3Cr_2O_8$	166.101
icsd_248351	O_6Ru_2Sr	162.75	icsd_010341	$BaCrF_6$	166.101
icsd_291234	MnO_6Sb_2	12.62	icsd_010342	CrF_6Sr	166.101
icsd_032730	$CaCoF_6Li$	15.87	icsd_014208	Cl_2Ni	12.58
icsd_032732	CaF_6LiNi	15.88	icsd_015558	$CrNaS_2$	12.58
icsd_032733	$F_6LiNiSr$	15.88	icsd_015939	Cl_2Co	12.62
icsd_062035	Cl_6CrNa_3	15.89	icsd_020372	$BiFeO_3$	166.101
icsd_073132	AlF_6LiPd	15.89	icsd_022106	Br_2Ni	12.58
icsd_073985	$CaCrF_6Li$	163.83	icsd_022108	I_2Ni	166.101
icsd_078748	$F_6GaLiPd$	15.89	icsd_022285	$HCoO_2$	12.58
icsd_183024	Cl_6MoNa_3	15.87	icsd_024594	LiO_2V	12.58
icsd_015901	Cl_2V	12.62	icsd_024595	$CrNaO_2$	166.101
icsd_016303	LiS_2V	12.62	icsd_025005	Ba_2NiO_6Te	166.1
icsd_022074	$Cl_9Cs_3Fe_2$	164.88	icsd_025723	$CrKS_2$	166.101
icsd_023591	H_2MnO_2	164.89	icsd_026305	NaS_2Ti	12.62
icsd_026233	$CrLiS_2$	12.62	icsd_028692	F_6KRu	12.58
icsd_028101	H_2NiO_2	164.89	icsd_028693	F_6RbRu	12.58
icsd_028779	F_6K_2Rh	12.62	icsd_028694	CsF_6Ru	12.58
icsd_028780	F_6Rb_2Rh	12.62	icsd_028783	F_3Ti	166.101
icsd_033673	I_2Mn	164.89	icsd_029011	FeO_2Tl	166.1
icsd_037327	Li_2MnO_2	164.89	icsd_029225	$CoLiO_2$	12.58
icsd_039512	As_2Mn_2Zn	12.6	icsd_030114	F_6NiSr	166.101
icsd_041789	$CaMn_2Sb_2$	12.6	icsd_031679	$CrNaSe_2$	166.101
icsd_041790	Mn_2Sb_2Sr	12.61	icsd_032551	$Fe_2Ga_2S_5$	12.61
icsd_041791	Bi_2CaMn_2	12.6	icsd_033752	Cl_2Mn	166.101
icsd_041792	As_2CaMn_2	164.89	icsd_035396	BaF_6Ni	12.62
icsd_041793	As_2Mn_2Sr	12.6	icsd_037157	$FeNaO_2$	12.58
icsd_044908	$LiTe_2Ti$	12.58	icsd_040267	$CrKO_2$	166.101
icsd_049017	$CaMn_2P_2$	12.6	icsd_041814	Sb_2V_3	12.58
icsd_049019	Mn_2P_2Sr	12.6	icsd_042158	F_6RhSr	166.101
icsd_052364	Br_2Co	12.58	icsd_043439	NaO_2Ti	12.58
icsd_052365	Br_2Fe	12.62	icsd_051207	$FeLiO_2$	166.101
icsd_052368	CoI_2	12.58	icsd_061276	F_6MnRb_2	12.58
icsd_052369	FeI_2	12.58	icsd_061692	$IrKLi_6O_6$	166.101
icsd_059230	Ga_2NiS_4	12.58	icsd_064764	$DCoO_2$	12.58
icsd_060250	Br_2Mn	164.89	icsd_067500	Br_2Mn	166.101
icsd_064831	Cl_2Fe	12.62	icsd_067701	Fe_2O_4Y	12.62
icsd_071421	Li_2NiO_2	164.89	icsd_071536	$CoK_2O_6Se_2$	12.58
icsd_071996	D_8FeMg_2Sr	164.89	icsd_071540	$K_2MnO_6Se_2$	166.101
icsd_072831	F_6NbRb_2	12.58	icsd_074030	Ba_2IrO_6Sr	166.101
icsd_072832	Cs_2F_6Nb	12.62	icsd_074680	$Cl_{12}OsS_2$	12.58
icsd_079007	$CrTe_2Tl$	164.89	icsd_076541	NaS_2V	12.62
icsd_086519	S_2V	12.58	icsd_076959	NiO	12.58
icsd_086520	Se_2V	12.62	icsd_077597	$NaSe_2V$	12.62
icsd_088722	CoO_2	12.58	icsd_085055	$Cr_2O_8Sr_3$	166.1
icsd_088940	H_2CoO_2	12.58	icsd_097758	$CrLiO_2$	166.101
icsd_095779	F_6IrK_2	12.62	icsd_108892	$Ni_3Pb_2Se_2$	12.62
icsd_100706	$FeGa_2S_4$	12.58	icsd_108893	$Ni_3S_2Tl_2$	12.58
icsd_152482	$Ba_3CaO_9Ru_2$	164.88	icsd_165117	$K_3Mn_2O_8$	166.101
icsd_159909	$Fe_2K_3NaO_8$	12.6	icsd_166489	KS_2Ti	12.58
icsd_182700	N_3V_2	164.89	icsd_170135	$CMnN_2$	166.101
icsd_240955	F_6IrRb_2	12.62	icsd_170347	NaO_2Ru	12.62
icsd_240956	Cs_2F_6Ir	12.62	icsd_280045	$Ba_3Mn_2O_8$	12.6
icsd_246906	Br_2V	12.58	icsd_291388	$Cs_2Cu_3F_{12}Sn$	12.62

TABLE S75. ICSD numbers, chemical formulas, and magnetic space groups (MSGs) for magnetic linear combinations of elementary band representation (LCEBR).

ICSD	Formula	MSG	ICSD	Formula	MSG
icsd_401026	$Cl_8Na_2Ti_3$	166.97	icsd_002782	Br_3CsMn	63.462
icsd_407802	Ba_2MnO_6Te	12.58	icsd_008193	BaS_3V	63.462
icsd_420137	NaO_2V	12.58	icsd_009704	Br_3MnRb	194.268
icsd_425834	$H_6Cl_2Cu_3O_6Zn$	12.62	icsd_010331	$BaMnO_3$	63.462
icsd_640140	$In_2Ni_3Se_2$	12.58	icsd_015011	Br_3NiRb	194.268
icsd_641350	KS_2Zr	12.58	icsd_015092	CsF_3Ni	63.463
icsd_670082	$AuCrO_2$	12.58	icsd_016360	$Ba_2Mn_2OSb_2$	194.271
icsd_670084	$AuFeO_2$	166.101	icsd_016361	$Ba_2Bi_2Mn_2O$	194.271
icsd_001462	O_3Ti_2	15.85	icsd_016773	AsTi	63.461
icsd_001473	O_3V_2	15.88	icsd_023874	$BaMnO_3$	63.463
icsd_005208	$CCoO_3$	167.103	icsd_024305	Cl_3CoRb	63.463
icsd_015840	Fe_2O_3	167.103	icsd_026453	CsI_3V	63.462
icsd_016649	F_3Ti	15.85	icsd_027511	Cl_3CoCs	63.464
icsd_016671	F_3Fe	15.89	icsd_029284	CPV_2	63.461
icsd_016672	CoF_3	167.103	icsd_029302	FeS	63.462
icsd_016673	F_3Ru	15.85	icsd_029305	CoS	63.462
icsd_025781	Cr_2O_3	167.106	icsd_029308	FeSe	63.457
icsd_025828	CrF_3	15.85	icsd_029310	NiSe	63.457
icsd_026629	F_3Mo	15.85	icsd_029313	NiS	194.268
icsd_028556	$CMnO_3$	167.103	icsd_042444	PV	63.463
icsd_030624	F_3V	15.85	icsd_042541	CoSe	63.462
icsd_030662	Ba_3NiO_4	15.89	icsd_042919	$CGeV_2$	194.271
icsd_034474	$BFeO_3$	15.89	icsd_043874	$CAsV_2$	63.461
icsd_043311	$BCrO_3$	15.85	icsd_049666	CrS	194.268
icsd_045060	BO_3V	15.89	icsd_049747	Cl_3RbTi	63.462
icsd_061067	$CNiO_3$	15.85	icsd_049748	Cl_3CsTi	63.462
icsd_100678	$CFeO_3$	15.85	icsd_049912	$Fe_2Ga_2S_5$	63.46
icsd_252432	LiO_3Os	167.103	icsd_052121	STi	194.268
icsd_402039	BO_3Ti	15.85	icsd_052509	TeV	63.462
icsd_094318	$BLiMnO_3$	174.135	icsd_056288	$HCoO_2$	63.457
icsd_036502	Ba_3FeN_3	11.53	icsd_058188	$AlTi_3$	63.461
icsd_072920	S_4V_3	11.53	icsd_058714	Be_2Mn	63.461
icsd_095740	$CBaF_2MnO_3$	176.145	icsd_058752	Be_2V	63.461
icsd_168997	FeO_4P	21.41	icsd_059371	Cl_3CsNi	194.268
icsd_002769	$BaFe_2O_4$	20.34	icsd_071010	$FeInO_3$	194.266
icsd_022092	Cl_3Ru	185.2	icsd_076218	MnSe	63.457
icsd_002064	Cl_3CsCu	36.174	icsd_076802	CCr_2Ge	63.461
icsd_002590	Br_3CrCs	186.205	icsd_084212	Cl_3CuRb	194.268
icsd_008105	$CrCsI_3$	186.205	icsd_103991	$GaTi_3$	63.461
icsd_010206	Cl_3CrCs	186.205	icsd_154258	CsI_3Ti	63.457
icsd_025578	F_6MnRb_2	36.175	icsd_155189	Cl_3CoTl	63.462
icsd_042493	NiS	186.205	icsd_157935	MnO_3Sr	63.459
icsd_043458	CoO	36.172	icsd_169572	NiS_2	63.465
icsd_044765	MnS	36.172	icsd_174041	Br_3CsFe	63.457
icsd_053528	FeS	36.176	icsd_181100	$CPTa_2$	63.461
icsd_060417	F_6K_2Mn	186.207	icsd_183361	CCr_2Si	63.465
icsd_076745	HCr	186.205	icsd_185562	NRu	63.462
icsd_091953	DCdClO	36.172	icsd_187133	AsFeLi	63.464
icsd_168369	MoN	186.205	icsd_191077	HTi	63.462
icsd_251820	CaFeOS	36.172	icsd_191172	MnSn	63.462
icsd_252146	CaCoOS	186.205	icsd_201829	Br_3CsV	63.462
icsd_262928	MnO	36.172	icsd_201830	Cl_3RbV	63.462
icsd_281495	$ClFeN_3O_3$	36.172	icsd_249387	$CCoN_2$	63.457
icsd_643594	MnSe	36.172	icsd_249388	CN_2Ni	194.268
icsd_043671	CRu	38.191	icsd_290431	N_2Ta	63.461
icsd_088670	$BaCoO_3$	38.191	icsd_300249	Cl_3CsFe	63.462
icsd_022091	Cl_3Ru	40.206	icsd_410394	$Cs_2F_6Ni_2$	63.463
icsd_002278	$CrCsF_4$	189.224	icsd_419223	$CFeN_2$	63.462
icsd_096248	$FeSb_2Y_6$	38.191	icsd_423829	Br_3CsNi	194.268
icsd_411152	$Li_5N_3Ni_3$	38.189	icsd_423830	CsI_3Ni	63.457
icsd_187196	GeMn	19.27	icsd_425293	$CrKO_2$	194.268
icsd_182351	N_4Ta_2	65.486	icsd_624986	$Co_{1.82}Se_{2.08}$	63.462
icsd_004068	Br_3Zr	63.462	icsd_633476	$Fe_{1.82}Se_{2.08}$	63.457
icsd_022090	Cl_3Ru	193.259	icsd_636809	$GeLaLi_2$	63.461
icsd_023163	Cl_3Zr	63.457	icsd_657109	$Co_{1.82}S_{2.08}$	63.462
icsd_023172	I_3Ti	63.462	icsd_659040	$Fe_{2.85}N_{1.14}$	63.462
icsd_023946	I_3Zr	63.462	icsd_670081	$AuCoO_2$	63.462
icsd_023947	HfI_3	193.259	icsd_670893	CMo	63.461
icsd_026069	Cl_3Ti	193.259	icsd_005250	FeSi	19.27
icsd_413691	Br_3Ru	63.462	icsd_016837	CrSi	19.25

TABLE S76. ICSD numbers, chemical formulas, and magnetic space groups (MSGs) for magnetic linear combinations of elementary band representation (LCEBR).

ICSD	Formula	MSG	ICSD	Formula	MSG
icsd_016838	MnSi	146.1	icsd_041209	F_2Pd	205.33
icsd_016839	CoSi	19.27	icsd_066939	O_2Ru	61.436
icsd_020309	AsNiS	19.27	icsd_166458	N_2Os	61.436
icsd_038843	NiSSb	198.9	icsd_024252	MnSe	160.67
icsd_042417	CrGe	19.27	icsd_029082	CoO	119.319
icsd_043054	FeGe	19.25	icsd_041258	FeN	119.319
icsd_053938	AsCoS	19.25	icsd_076205	MnS	44.231
icsd_093898	NiPS	19.27	icsd_167870	NTc	44.231
icsd_093901	AsNiSe	198.9	icsd_168901	BTc	160.67
icsd_093902	NiSbSe	19.27	icsd_169407	CSc	44.231
icsd_100568	F_2Pd	198.9	icsd_169409	GeSc	160.67
icsd_624862	CoSSb	19.25	icsd_181079	CrN	160.67
icsd_002896	$CuO_6S_2Tl_2$	2.4	icsd_181324	MnTe	44.231
icsd_006240	Ba_2CuO_6Te	2.6	icsd_183168	CTc	119.319
icsd_018115	$As_2CuO_8Zn_2$	2.4	icsd_186876	MoP	160.67
icsd_023334	MnP_4	2.6	icsd_192816	AsLiMn	44.231
icsd_036208	$Fe_2O_7P_2$	2.6	icsd_236783	NV	160.67
icsd_036514	CuF_6Sn	2.4	icsd_236787	MnN	160.67
icsd_039784	Br_3Ti	2.6	icsd_671343	CrSe	160.67
icsd_050444	$Cs_4CuO_7Si_2$	2.4	icsd_671386	SeV	44.231
icsd_051505	AgF_6Sn	2.4	icsd_671387	TeV	160.67
icsd_059585	$FeNa_4O_4$	2.4	icsd_015246	CoF_3K	166.101
icsd_059721	$AsBiMnO_5$	2.6	icsd_015423	F_3KMn	65.486
icsd_062544	$AuCuF_5$	2.4	icsd_015424	F_3FeK	166.101
icsd_062676	$CrNa_4O_4$	2.4	icsd_015426	F_3KNi	166.101
icsd_063058	$As_2CuNa_4O_8$	2.4	icsd_023167	Cl_3MnTl	65.486
icsd_065186	$AgF_{12}Sb_2$	2.4	icsd_028145	F_3KV	123.345
icsd_066023	$Cl_{12}Te_4W_2$	2.4	icsd_028146	F_3RbV	123.345
icsd_069994	H_2O_5SeV	2.4	icsd_030612	F_3Mo	65.486
icsd_072461	$H_6CuN_4O_4$	2.4	icsd_030613	F_3Ta	166.101
icsd_074682	$Cl_{12}OsTe_2$	2.4	icsd_043722	F_3MnRb	123.345
icsd_078789	Cl_6ISe_6W	2.4	icsd_044616	RuSi	166.101
icsd_079879	$AgBi_2F_{12}$	2.4	icsd_049583	CsF_3Fe	166.101
icsd_080430	$KMnO_8Se_2$	2.4	icsd_049586	F_3FeRb	166.101
icsd_084620	Cl_5Mo	2.4	icsd_058151	AlRh	65.486
icsd_085404	$CuK_6O_8Si_2$	2.4	icsd_060611	F_3NaV	166.101
icsd_085405	$CuO_7Rb_4Si_2$	2.4	icsd_069360	O_3RuSr	166.101
icsd_087958	$H_4FeK_2O_{10}S_2$	2.4	icsd_071994	MoO_3Sr	166.101
icsd_092916	$AsBiNiO_5$	2.6	icsd_073166	F_3PdRb	65.486
icsd_096783	$H_4K_2MnO_{10}Se_2$	2.4	icsd_073167	F_3KPd	65.486
icsd_098683	$H_4CoNa_2O_{10}Se_2$	2.4	icsd_102423	CoGa	65.486
icsd_098684	$H_4Na_2NiO_{10}Se_2$	2.4	icsd_103950	GaRu	65.486
icsd_098686	$H_4CoK_2O_{10}Se_2$	2.4	icsd_109076	O_3SrTc	123.345
icsd_099580	$Co_2Na_6O_6$	2.4	icsd_168836	$H_2Mg_{0.25}Ti_{0.75}$	166.97
icsd_156225	$H_4Ca_2MnO_{10}P_2$	2.4	icsd_168900	BTc	65.486
icsd_166313	NaO_6Si_2Ti	2.6	icsd_168902	$CaMnO_3$	123.345
icsd_171007	$Ca_2Cl_2CuO_{10}Te_4$	2.4	icsd_236833	NNi	166.101
icsd_171656	F_6O_2Rh	2.4	icsd_237730	BaO_3Os	65.486
icsd_172335	$C_2CuF_6O_6S_2$	2.4	icsd_671082	CaO_3Tc	123.345
icsd_173748	$F_2O_7Te_2V_2$	2.6	icsd_671086	BaO_3Tc	123.345
icsd_174291	Ba_2BiIrO_6	2.4	icsd_671397	F_3NiRb	65.486
icsd_196024	$CMnO_3$	2.6	icsd_020212	GeV_3	167.105
icsd_196300	FeSe	2.6	icsd_105639	PbV_3	167.105
icsd_237763	$BaFe_2O_8P_2$	2.6	icsd_106097	SnV_3	167.105
icsd_240930	$Cu_2Na_2O_{11}Si_4$	2.6	icsd_009864	MnO	139.537
icsd_409506	$Cs_6NiO_8Si_2$	2.4	icsd_009865	CoO	166.101
icsd_411522	$F_{12}MnSb_2$	2.4	icsd_009866	NiO	71.536
icsd_415445	O_5PSnV	2.4	icsd_018007	MnS	139.537
icsd_415768	Cl_8NW_2	2.4	icsd_024251	MnSe	139.537
icsd_418858	$Br_2CoO_3Sb_2$	2.6	icsd_027856	FeO	71.536
icsd_423336	Cs_4FeO_3	2.6	icsd_037412	CrN	139.537
icsd_423462	Br_5W	2.4	icsd_040125	OTi	71.536
icsd_424465	$Br_{10}CoY_6$	2.4	icsd_065410	F_2Ti	71.536
icsd_424841	$CoI_{10}Y_6$	2.4	icsd_076240	MnTe	166.101
icsd_428633	$AsBiCoO_5$	2.6	icsd_167854	NTc	166.101
icsd_015991	MnS_2	61.436	icsd_186838	CrO_2	71.536
icsd_024020	$MnSe_2$	61.436	icsd_191169	MnSn	71.536
icsd_024021	$MnTe_2$	205.33	icsd_075401	$CCuFKO_3$	26.7
icsd_040328	NiS_2	205.33	icsd_031189	AsCoS	29.99
icsd_040330	$NiSe_2$	61.436	icsd_002257	$HCrO_2$	31.125

TABLE S77. ICSD numbers, chemical formulas, and magnetic space groups (MSGs) for magnetic linear combinations of elementary band representation (LCEBR).

ICSD	Formula	MSG	ICSD	Formula	MSG
icsd_002258	$DCrO_2$	31.125	icsd_016013	ClFeO	59.407
icsd_023425	$CoGeNa_2O_4$	31.123	icsd_025657	ClOTi	59.411
icsd_040044	CoSSb	31.127	icsd_027010	BrOV	59.41
icsd_047101	$MnNa_5O_4$	31.127	icsd_027092	BrCrO	59.409
icsd_071177	H_2KMnO_5P	31.125	icsd_028119	Br_3Ru	59.411
icsd_087325	$HFeO_2$	31.127	icsd_059345	NaO_5V_2	59.409
icsd_161305	Li_2MnO_4Si	31.125	icsd_069659	BrCrS	59.41
icsd_161306	$FeLi_2O_4Si$	31.123	icsd_074648	I_3Zr	59.407
icsd_420003	$DFeO_2$	31.127	icsd_082689	CaO_5V_2	59.41
icsd_670672	Li_2MnS_4Sn	31.127	icsd_088639	LiO_5V_2	59.409
icsd_015009	AsFe	33.144	icsd_165626	$BaCrS_2$	59.407
icsd_015057	FeP	33.144	icsd_173784	I_3Ti	59.407
icsd_015065	AsCo	33.148	icsd_195025	Fe_2OS_2Sr	59.411
icsd_023527	MnN_2Si	33.146	icsd_195027	Fe_2OSe_2Sr	59.411
icsd_023528	$GeMnN_2$	33.146	icsd_260162	Br_3Tc	59.407
icsd_027117	$FeNaO_2$	33.148	icsd_414041	Cl_3Ru	59.411
icsd_042445	AsV	33.148	icsd_428170	$BaFe_2OS_2$	59.411
icsd_000284	MgO_3V	36.174	icsd_009965	CV_2	60.42
icsd_001544	$HFeO_2$	36.174	icsd_015522	Cl_3CuRb	60.422
icsd_002596	CrI_2	36.174	icsd_020365	F_2Mn	60.422
icsd_052692	BaS_3V	36.176	icsd_023382	$CrCsI_3$	60.417
icsd_068459	H_2CuO_2	36.176	icsd_042979	Mn_2N	60.425
icsd_159030	$CaIrO_3$	36.174	icsd_096077	Fe_2O_3	60.424
icsd_050648	NbS_2	38.189	icsd_006277	AgF_2	61.436
icsd_004327	CuI_2O_6	4.9	icsd_291504	MnS_2	61.436
icsd_008010	FeI_4Rb_2	4.9	icsd_000495	MnO_3Se	62.448
icsd_093022	O_7P_2V	4.9	icsd_000496	CoO_3Se	62.441
icsd_670113	$CuFO_2$	4.7	icsd_000497	NiO_3Se	62.446
icsd_430557	Fe_2O_3	41.211	icsd_000498	CuO_3Se	62.446
icsd_071339	$NbSe_2$	42.221	icsd_000500	CoO_3Te	62.441
icsd_072198	Se_2Ta	42.221	icsd_000990	RuSb	62.444
icsd_095729	NbO	47.252	icsd_004063	Cl_3FeK	62.449
icsd_039871	$HCsMnO_{10}P_3$	5.15	icsd_004064	Br_3FeK	62.441
icsd_059910	CsP_2S_7V	5.15	icsd_004404	CoF_3Na	62.448
icsd_075180	As_2FeLiO_7	5.13	icsd_005418	CrP	62.443
icsd_084683	B_2BaCuO_5	5.15	icsd_009008	F_3NaNi	62.441
icsd_091754	$CrKP_2S_7$	5.15	icsd_015621	F_3MnNa	62.446
icsd_091756	KP_2S_7V	5.15	icsd_020228	MnO_2	62.447
icsd_260893	$CrCsP_2S_7$	5.15	icsd_022303	O_2V	62.448
icsd_025754	$CuGeO_3$	51.294	icsd_023168	Cl_3MnTl	62.446
icsd_089669	CuO_3Si	51.294	icsd_023589	AsCr	62.443
icsd_015087	$H_4Cl_2CuO_2$	53.328	icsd_024564	SV	62.449
icsd_009136	Cl_4MnNa_2	55.358	icsd_026420	I_3MnTl	62.446
icsd_022046	$GeMn_2O_4$	55.358	icsd_026422	FeI_3Tl	62.443
icsd_035130	$Ca_2Mn_2O_5$	55.356	icsd_029338	CuO_3Te	62.448
icsd_035219	$CaMnO_{2.5}$	55.356	icsd_030413	AsFe	62.444
icsd_090183	$Mn_2O_5Sr_2$	55.356	icsd_030450	BCo	62.449
icsd_400264	Cl_4Na_2Ti	55.353	icsd_031453	$BaMnS_2$	62.449
icsd_005071	$NiSe_2$	58.393	icsd_031820	F_3KMn	62.446
icsd_015027	FeP_2	58.398	icsd_032710	Cl_3KMn	62.441
icsd_015467	Cl_2Cr	58.398	icsd_035008	FeS	62.446
icsd_016895	CCo_2	58.396	icsd_035218	$CaMnO_3$	62.447
icsd_025680	$FeSe_2$	58.393	icsd_036217	Br_3FeTl	62.443
icsd_034307	F_2Ni	58.398	icsd_038636	$FNaNbO_2$	62.447
icsd_041123	$H_4O_4V_2$	58.398	icsd_042441	Br_3KMn	62.446
icsd_048007	LiO_2Ru	58.398	icsd_042446	AsV	62.449
icsd_076826	CFe_2	58.395	icsd_042577	AsRu	62.444
icsd_084619	O_2Ru	58.393	icsd_043248	FeP	62.444
icsd_155832	CrO_2	58.398	icsd_043494	SiTi	62.445
icsd_172908	$C_2H_2N_4Ni$	58.398	icsd_048026	AsCo	62.449
icsd_236413	$C_2H_2CoN_4$	58.397	icsd_051291	CaO_3Ru	62.441
icsd_419222	$C_2H_2FeN_4$	58.393	icsd_052705	$CaMnSb_2$	62.449
icsd_643441	MnS_2	58.398	icsd_056697	O_3RuSr	62.447
icsd_001981	ClOV	59.41	icsd_066279	$CrGaSe_3$	62.448
icsd_004086	ClCrO	59.409	icsd_068981	F_3FeNa	62.446
icsd_004202	Cu_2MgO_3	59.409	icsd_074601	CrS_3Sb	62.447
icsd_010419	BrOTi	59.409	icsd_075469	Br_3FeIn	62.443
icsd_015094	$CaCu_2O_3$	59.41	icsd_075470	Br_3InMn	62.446
icsd_015768	$LiMnO_2$	59.407	icsd_076630	BMn	62.443
icsd_015769	$MnNaO_2$	59.407	icsd_081056	CaO_3V	62.448

TABLE S78. ICSD numbers, chemical formulas, and magnetic space groups (MSGs) for magnetic linear combinations of elementary band representation (LCEBR).

ICSD	Formula	MSG	ICSD	Formula	MSG
icsd_084866	$CrSbSe_3$	62.446	icsd_670121	$CuMgO_2$	67.506
icsd_084948	$HMnO_2$	62.446	icsd_166017	As_2CaFe_2	69.523
icsd_091273	N_2NiSr_2	62.444	icsd_039528	Br_7FeSe	7.24
icsd_093161	CrTe	62.443	icsd_200680	$CoGeNa_2O_4$	7.24
icsd_093835	FeO_3Tl	62.446	icsd_238234	$FeGeLi_2S_4$	7.26
icsd_109041	$DFeO_2$	62.446	icsd_238236	$FeLi_2S_4Sn$	7.26
icsd_109139	PRu	62.444	icsd_281242	I_6K_2Re	7.24
icsd_151925	$ClMnS_2Sb$	62.444	icsd_010038	$BaMn_2O_3$	71.535
icsd_153239	$CaMnO_{2.98}$	62.448	icsd_015127	CuO_3Sr_2	71.536
icsd_159433	$CaIrO_3$	62.448	icsd_016216	Ca_2CuO_3	71.536
icsd_160454	$BiCrO_3$	62.446	icsd_024380	Cl_2OV	71.536
icsd_162895	$BiFeO_3$	62.448	icsd_024381	Br_2OV	71.536
icsd_164775	CaO_3Rh	62.447	icsd_025001	$CuLi_2O_2$	71.536
icsd_172156	$BiClMnS_2$	62.444	icsd_025697	$CsFeS_2$	71.535
icsd_172784	$BrMnSbSe_2$	62.444	icsd_068700	$FeLi_4N_2$	71.536
icsd_172790	$CaMoO_3$	62.447	icsd_078012	AlF_5Fe	71.536
icsd_183450	O_3SrTc	62.441	icsd_251018	FeO_3Sr_2	71.536
icsd_185586	$CrInO_3$	62.441	icsd_633207	$FeRbS_2$	71.535
icsd_193272	Bi_3Co	62.447	icsd_065453	K_2MnS_2	72.542
icsd_196446	IrO_3Sr	62.448	icsd_065454	$MnRb_2S_2$	72.542
icsd_237731	O_3OsSr	62.447	icsd_065455	Cs_2MnS_2	72.542
icsd_237732	CaO_3Os	62.446	icsd_065456	K_2MnSe_2	72.542
icsd_238293	$BiMnO_3$	62.446	icsd_065457	$MnRb_2Se_2$	72.542
icsd_238591	MnS	62.449	icsd_065458	Cs_2MnSe_2	72.542
icsd_238684	CaFeOSe	62.444	icsd_065459	K_2MnTe_2	72.542
icsd_238834	CrO_3Tl	62.447	icsd_065460	$MnRb_2Te_2$	72.542
icsd_239321	$HFeO_2$	62.444	icsd_065461	Cs_2MnTe_2	72.542
icsd_245840	$CaCrO_3$	62.448	icsd_067386	$CoNa_2S_2$	72.542
icsd_247467	$BiCoO_3$	62.446	icsd_067387	CoK_2S_2	72.542
icsd_252431	NaO_3Os	62.448	icsd_067388	$CoRb_2S_2$	72.542
icsd_261341	CaO_3Tc	62.448	icsd_067389	$CoCs_2S_2$	72.542
icsd_425310	B_2Fe	62.443	icsd_067390	CoK_2Se_2	72.542
icsd_643539	$MnSb_2Sr$	62.449	icsd_067391	$CoRb_2Se_2$	72.542
icsd_652036	SeTi	62.449	icsd_067392	$CoCs_2Se_2$	72.542
icsd_670832	CFe_2Si	62.447	icsd_624264	$CoNa_2Se_2$	72.542
icsd_016217	CuO_2Sr	63.463	icsd_174205	MoO_3Sr	74.554
icsd_024885	$HFeO_2$	63.459	icsd_183451	O_3SrTc	74.554
icsd_025524	$CaIrO_3$	63.464	icsd_670124	CuO_2Pb	74.558
icsd_030603	BCr	63.461	icsd_670341	$CaMnO_3$	74.559
icsd_036123	NiO_2Sr	63.463	icsd_006179	$CCuO_3$	8.34
icsd_042952	BV	63.465	icsd_095439	Ca_2CoO_3	8.34
icsd_054129	Cu_4O_8	63.463	icsd_095440	CoO_2	8.34
icsd_063228	BaS_3V	63.462	icsd_168320	$BiFeO_3$	8.34
icsd_150913	CuO_2	63.463	icsd_169981	$HNiO_2$	8.32
icsd_161460	$CCuN_2$	63.462	icsd_000415	Ga_2MnSe_4	82.39
icsd_180910	O_3RuSr	63.457	icsd_052961	$CoGa_2S_4$	82.39
icsd_187134	FeLiP	63.459	icsd_152909	Ga_2MnS_4	82.39
icsd_192141	F_3NaNi	63.462	icsd_103995	Ga_3Ti_2	10.44
icsd_192148	CoF_3Na	63.464	icsd_018307	O_5SV	85.59
icsd_251575	F_3FeNa	63.462	icsd_024894	MoO_5P	85.62
icsd_252147	BaCoOS	63.459	icsd_056181	HTi	13.69
icsd_613898	BFe	63.459	icsd_023081	$BaFe_2S_4$	12.6
icsd_656056	Cs_2NiP_2	63.464	icsd_033573	CuO_6Sr_2Te	87.75
icsd_658704	Bi_2Cs_2Ni	63.457	icsd_067826	$IrNa_4O_4$	87.75
icsd_670104	$BaCuO_2$	63.463	icsd_077697	O_5Ti_4	12.6
icsd_670348	$CaMnO_3$	63.464	icsd_174033	$O_{1.25}Ti$	12.6
icsd_001165	Cl_4Os	65.486	icsd_194696	MgO_6OsSr_2	12.62
icsd_023265	Mn_2S_4Sn	65.486	icsd_238713	$BaFe_2Se_4$	12.6
icsd_033865	Br_4Li_2Mn	65.486	icsd_001410	$FeNa_4O_3$	9.39
icsd_073227	Cl_4CoLi_2	65.486	icsd_010501	$CoNa_4O_3$	9.39
icsd_082199	Br_4FeLi_2	65.486	icsd_023174	$CaCrF_5$	9.37
icsd_099041	Cu_2O_3Sr	65.483	icsd_069757	CuO	9.39
icsd_174117	CuF_4K_2	65.486	icsd_169098	MoO_5P	9.37
icsd_174209	F_7KTi_2	65.487	icsd_192515	$BiFeO_3$	9.39
icsd_261512	$Fe_2O_5Sr_3$	65.484	icsd_033768	$FeNaO_2$	92.113
icsd_075515	$BaCoS_2$	67.503	icsd_023173	F_6Li_2Mo	18.19
icsd_163555	FeSe	67.503	icsd_081589	$H_4Cl_2CuO_4Pb_2$	99.167
icsd_163916	AsFFeSr	67.503	icsd_152276	O_3PbV	99.167
icsd_168206	AsFeLi	67.503	icsd_157833	$BiCoO_3$	99.167
icsd_186504	AsCaFFe	67.503	icsd_188466	$BiFeO_3$	35.167

TABLE S79. ICSD numbers, chemical formulas, and magnetic space groups (MSGs) for magnetic linear combinations of elementary band representation (LCEBR).

ICSD	Formula	MSG	ICSD	Formula	MSG
icsd_004189	CuO_4W	2.6	icsd_097745	MnO_6Sr_2W	14.75
icsd_030117	CuF_6Zr	2.4	icsd_098732	Ca_2CoO_6W	14.75
icsd_037027	Ba_2LaO_6Ru	2.4	icsd_098733	Ca_2NiO_6W	14.75
icsd_051506	AgF_6Ti	2.4	icsd_100793	Ba_2LaO_6Ru	14.79
icsd_078869	$CuF_{11}NaZr_2$	2.4	icsd_160372	La_2NaO_6Ru	14.75
icsd_092852	$CoLi_2O_8W_2$	2.4	icsd_170175	La_2NaO_6Os	14.75
icsd_092853	$Li_2NiO_8W_2$	2.4	icsd_172591	FeO_6Sr_2Ta	14.75
icsd_092854	$CuLi_2O_8W_2$	2.4	icsd_173491	CoO_6ReSr_2	14.79
icsd_174140	Ba_2IrLaO_6	2.4	icsd_203219	La_2LiMoO_6	14.79
icsd_200533	$CuFNbO_3$	2.4	icsd_238311	O_6OsSr_2Y	14.79
icsd_249777	$Cd_2CuO_8P_2$	2.4	icsd_247998	Ca_2MnO_6Re	14.79
icsd_280299	$H_8CdCl_4CuO_4$	2.4	icsd_291608	Ca_2O_6OsSc	14.75
icsd_159097	$LaMnNaO_6W$	4.7	icsd_413634	$IrLa_2NaO_6$	14.79
icsd_237487	$FeLaNaO_6W$	4.7	icsd_414605	$IrLa_2LiO_6$	14.79
icsd_238785	$La_2Mn_2O_{12}Rb_2W_2$	4.7	icsd_416199	La_2LiO_6Os	14.79
icsd_238786	$K_2La_2Mn_2O_{12}W_2$	4.7	icsd_099370	$CoLaO_3$	15.89
icsd_238788	$K_2Mn_2O_{12}W_2Y_2$	4.9	icsd_051698	CdO_3Ti	26.7
icsd_238789	$La_2Mn_2Na_2O_{12}W_2$	4.7	icsd_236365	MnO_3Y	31.125
icsd_238791	$Mn_2Na_2O_{12}W_2Y_2$	4.7	icsd_023822	FeO_3Y	33.148
icsd_238793	$Mn_2O_{12}Rb_2W_2Y_2$	4.9	icsd_157925	HLaNiSn	62.444
icsd_068143	AgP_2Se_6V	5.13	icsd_057007	C_2CoY	38.189
icsd_425760	Ag_2FeS_4Si	7.26	icsd_617417	C_2CoLu	38.19
icsd_023476	$CrNb_2Se_4$	8.34	icsd_617756	C_2FeLu	38.191
icsd_645393	Nb_2Se_4Ti	8.34	icsd_670125	CuO_2Pt	53.326
icsd_028909	CrO_3Y	10.46	icsd_073399	$Cu_2La_2O_5$	55.359
icsd_150279	$AuCrTe_4$	10.42	icsd_077943	$CuLaO_{2.5}$	55.359
icsd_035044	$Cr_2Nb_2Se_{10}$	11.52	icsd_008146	LaO_3Ti	62.441
icsd_060759	CuF_2O_3W	11.5	icsd_008150	O_3TiY	62.446
icsd_066513	$FeTaTe_3$	11.52	icsd_009938	$CrLaO_3$	62.446
icsd_078041	$F_7MnTlZr$	11.52	icsd_014192	$CrLaOS_2$	62.446
icsd_078042	$F_7MnRbZr$	11.53	icsd_016280	$LaMnO_3$	62.447
icsd_084825	$CoPZr_2$	11.53	icsd_020079	BCoRe	62.441
icsd_246091	Ca_2MnO_6Ta	11.54	icsd_027285	$FeLuO_3$	62.446
icsd_252429	H_3ClCuO_3Zn	11.5	icsd_028255	$FeLaO_3$	62.446
icsd_020661	$FeSc_2Si_2$	12.61	icsd_039562	PVZr	62.444
icsd_077912	CoO_6Pb_2W	12.58	icsd_041893	B_2CoNb	62.441
icsd_174141	Ba_2IrLaO_6	12.58	icsd_043260	FeO_3Y	62.446
icsd_427606	$FeLa_2O_2Se_2$	12.62	icsd_049729	FePTa	62.443
icsd_617825	$CFe_2Si_2Y_2$	12.61	icsd_051123	$CrLaS_3$	62.446
icsd_670065	$AgMnO_2$	12.62	icsd_053024	HfMnSi	62.444
icsd_670093	$AuMnO_2$	12.62	icsd_053189	CrNbP	62.443
icsd_670115	$CuHgO_2$	12.62	icsd_056617	MnO_3Y	62.447
icsd_008128	$FeNbO_4$	13.67	icsd_063520	LaO_3V	62.446
icsd_015192	FeO_4W	13.68	icsd_076236	MnSiZr	62.444
icsd_015850	MnO_4W	13.68	icsd_076346	FeScSi	62.445
icsd_015851	CoO_4W	13.67	icsd_085141	CrO_3Sc	62.441
icsd_015852	NiO_4W	13.67	icsd_086280	FeHfP	62.443
icsd_036456	$Ag_{0.5}Cr_{0.5}PS_3$	13.68	icsd_088387	CdO_3V	62.448
icsd_169005	CuO_4W	13.65	icsd_095577	O_3VY	62.446
icsd_170685	MnO_4Re	13.69	icsd_097805	GeMnY	62.444
icsd_202045	$Ag_{0.5}PS_3V_{0.5}$	13.68	icsd_109352	CrO_3Y	62.446
icsd_009390	CrO_6Ta_2	14.79	icsd_155834	CoO_3Y	62.441
icsd_049500	O_6RuSr_2Y	14.75	icsd_160376	$LuMnO_3$	62.447
icsd_051615	Ca_2MnO_6W	14.75	icsd_164459	$CoLaO_3$	62.448
icsd_073738	$CoTaTe_2$	14.78	icsd_172052	$CoLuO_3$	62.448
icsd_073739	$CoNbTe_2$	14.78	icsd_251093	$CrLuO_3$	62.446
icsd_075596	$IrLa_2O_6Zn$	14.79	icsd_260794	PtSiTi	62.445
icsd_079492	$IrLa_2MgO_6$	14.79	icsd_409926	GePdTi	62.449
icsd_088152	IrO_6ScSr_2	14.79	icsd_601849	CoLuSi	62.446
icsd_088153	Ba_2IrO_6Sc	14.75	icsd_601850	CoSnY	62.447
icsd_088154	IrO_6Sr_2Y	14.79	icsd_601861	CoGeLu	62.446
icsd_088155	Ba_2IrO_6Y	14.79	icsd_601862	CoLuSn	62.449
icsd_088156	Ba_2IrLaO_6	14.79	icsd_610089	AsCoNb	62.441
icsd_088158	Ba_2IrLuO_6	14.79	icsd_610502	AsFeNb	62.449
icsd_088522	La_2MgO_6Rh	14.75	icsd_610528	AsFeTa	62.443
icsd_088523	La_2O_6RhZn	14.79	icsd_613324	B_2CoTa	62.441
icsd_093880	$AgCuO_2$	14.75	icsd_613388	BCoW	62.443
icsd_095517	FeO_6Sr_2W	14.79	icsd_623231	CoGaY	62.447
icsd_097487	La_2LiO_6Ru	14.75	icsd_623439	CoGeHf	62.449
icsd_097662	CoO_6Sr_2W	14.79	icsd_623611	CoGeTa	62.444

TABLE S80. ICSD numbers, chemical formulas, and magnetic space groups (MSGs) for magnetic linear combinations of elementary band representation (LCEBR).

ICSD	Formula	MSG	ICSD	Formula	MSG
icsd_623685	CoGeZr	62.449	icsd_191362	$CoLaO_6Sr_2$	71.536
icsd_623786	CoHfP	62.443	icsd_191363	CoO_6Sr_2Zr	71.536
icsd_624322	CoNbSi	62.449	icsd_191629	La_2NiO_6Zr	71.536
icsd_624621	CoPSc	62.446	icsd_191630	$HfLa_2NiO_6$	71.536
icsd_624977	CoScSn	62.446	icsd_238076	$Ag_2Ba_2CoO_2Se_2$	71.536
icsd_625144	CoSiZr	62.446	icsd_623793	Co_2HfSi_2	71.535
icsd_626229	$CrLaSe_3$	62.443	icsd_625135	Co_2Si_2Zr	71.535
icsd_626529	CrPZr	62.444	icsd_633666	Fe_2Si_2Zr	139.536
icsd_632166	FeGeZr	62.443	icsd_634333	Ga_4HfV_2	71.535
icsd_632827	FeNbSi	62.445	icsd_635647	Ga_4V_2Zr	69.523
icsd_633568	FeSiTa	62.443	icsd_051014	MnO_8Re_2	2.4
icsd_633674	FeSiZr	62.444	icsd_051015	CoO_8Re_2	2.4
icsd_648877	PdSiTi	62.445	icsd_164936	$CrLaO_6Te$	15.87
icsd_085926	$LaMnSi_2$	63.465	icsd_030116	CuF_6Zr	148.17
icsd_195899	$AsCo_2LaN$	63.461	icsd_152678	Ba_2IrLaO_6	2.4
icsd_632049	$FeGe_2La$	63.461	icsd_155549	Ba_2LaO_6Ru	148.17
icsd_632434	$FeLaSi_2$	63.459	icsd_262503	$C_6Ag_3KMnN_6$	5.15
icsd_670675	$AlTi_2Zr$	63.465	icsd_024797	$AgCrS_2$	8.32
icsd_009389	OTi_2Zr	65.483	icsd_024799	$AgCrSe_2$	8.32
icsd_035337	MnO_6Pt_3	65.486	icsd_084639	CrN_2W	160.67
icsd_035338	CoO_6Pt_3	65.485	icsd_605002	$AgCrTe_2$	8.32
icsd_180434	AsFeLaO	67.503	icsd_605619	$AgNiTe_2$	8.32
icsd_068795	$BaNiO_5Y_2$	71.536	icsd_173552	$C_6Ag_3FeN_6$	12.58
icsd_613131	B_4Co_4La	13.67	icsd_032731	$CdCoF_6Li$	15.87
icsd_009294	NiO_6Sr_2W	12.62	icsd_039666	Cl_6FeZr	15.87
icsd_078677	FeO_6Sr_2W	12.62	icsd_039817	Cl_6FeHf	163.81
icsd_095518	Ba_2FeO_6W	12.62	icsd_240281	$Ba_3NiO_9Ta_2$	12.58
icsd_150702	FeO_6ReSr_2	12.62	icsd_004149	$AgCrO_2$	166.101
icsd_190593	CoO_6Sr_2W	12.62	icsd_031919	$AgFeO_2$	166.101
icsd_192327	$CoNbO_6Sr_2$	12.62	icsd_099369	$CoLaO_3$	15.85
icsd_262352	$Co_{0.5}O_3Re_{0.5}Sr$	12.62	icsd_042650	$NbS_2V_{0.333}$	20.31
icsd_075318	$BBaCuLaO_5$	100.174	icsd_042687	$FeNb_3S_6$	20.31
icsd_042534	Ag_2FeS_4Sn	23.51	icsd_624304	$CoNb_3Se_6$	20.34
icsd_192470	$AgFe_2GaTe_4$	121.327	icsd_626392	$CrNb_3S_6$	20.34
icsd_056263	$AgFeS_2$	43.226	icsd_626398	$CrNb_3Se_6$	20.34
icsd_051261	$ClCuLaO_7Ta_2$	47.252	icsd_626633	CrS_6Ta_3	20.34
icsd_064639	$Ba_2Cu_2LaO_8Ta$	123.347	icsd_626727	$CrSe_6Ta_3$	20.34
icsd_074164	$Cu_2O_7Sr_2TlY$	123.347	icsd_633323	FeS_6Ta_3	20.33
icsd_075720	Ba_2CuHgO_4	123.345	icsd_643472	MnS_6Ta_3	20.34
icsd_075725	$Ba_2CaCu_2HgO_6$	123.347	icsd_645098	Nb_3NiSe_6	182.182
icsd_088032	$ClCuLaNb_2O_7$	47.252	icsd_645331	Nb_3S_6Ti	20.33
icsd_088033	$BrCuLaNb_2O_7$	47.252	icsd_645338	Nb_3S_6V	20.33
icsd_016496	CrNNb	59.407	icsd_651970	Se_6Ta_3V	182.183
icsd_080798	$ClFeO_4W$	67.503	icsd_080029	MnN_2W	186.205
icsd_085853	FeLaSi	59.407	icsd_023577	FeGeHf	38.191
icsd_088209	GeLuTi	59.407	icsd_042060	CrNbSi	38.191
icsd_191256	CrN_2Nb	67.503	icsd_042061	CrGeNb	38.191
icsd_237385	AsCrLaO	59.407	icsd_054566	Bi_2CoHf_6	38.189
icsd_262356	$As_2Co_2O_6Sc_2Sr_4$	67.506	icsd_090081	$FeSc_6Te_2$	38.191
icsd_262357	$Co_2O_6P_2Sc_2Sr_4$	59.407	icsd_096247	$FeSb_2Sc_6$	38.191
icsd_624027	CoLaSi	67.503	icsd_150575	Al_2CoZr_6	38.191
icsd_657914	$FeLaSb_2$	67.503	icsd_041460	Co_6Ge_6Zr	191.241
icsd_657919	$CoLaSb_2$	67.503	icsd_155117	Ge_6HfMn_6	65.483
icsd_002575	O_6V_2W	136.502	icsd_604198	$FePb_3Zr_5$	63.464
icsd_015306	CrO_6Ta_2	58.398	icsd_002786	$AgFeO_2$	194.268
icsd_020314	Cr_2O_6W	136.502	icsd_057984	AlMnPt	63.462
icsd_023600	O_6Ta_2V	136.499	icsd_080373	C_2CrSc	194.266
icsd_040337	FeO_6Ta_2	58.398	icsd_081488	FeN_2W	63.462
icsd_061198	NiO_6Ta_2	136.501	icsd_156263	GaPtTi	63.462
icsd_083367	CuO_6Ta_2	136.499	icsd_163350	AlPtTi	63.462
icsd_166673	CoO_6Ta_2	58.398	icsd_164891	Ge_3LaV	63.462
icsd_173874	Cr_2O_6Re	136.501	icsd_172878	$Ag_3Ni_2O_4$	63.461
icsd_075384	CrF_6Nb	69.524	icsd_180888	$AgCoO_2$	63.464
icsd_092989	AsTiZr	71.536	icsd_261608	$AgCoO_2$	63.461
icsd_168330	$Co_2La_2O_3Se_2$	71.536	icsd_103606	FePtSb	19.27
icsd_191357	CrO_6Sr_2Zr	71.536	icsd_181053	$Cd_{0.75}Cr_{0.25}Te$	160.67
icsd_191358	$CrHfO_6Sr_2$	71.536	icsd_181055	$Cd_{0.25}Cr_{0.75}Te$	160.67
icsd_191359	O_6Sr_2VZr	71.536	icsd_186189	$Cr_{0.25}TeZn_{0.75}$	111.255
icsd_191360	HfO_6Sr_2V	71.536	icsd_054465	AuMnSn	44.231
icsd_191361	CoO_6Sr_2Y	71.536	icsd_057421	MnPtSb	160.67

TABLE S81. ICSD numbers, chemical formulas, and magnetic space groups (MSGs) for magnetic linear combinations of elementary band representation (LCEBR).

ICSD	Formula	MSG	ICSD	Formula	MSG
icsd_083928	FeNbSb	119.319	icsd_030379	$CuMnO_2$	12.62
icsd_102552	CoNbSn	44.231	icsd_035634	FeS_4V_2	12.62
icsd_104955	MnPtSn	160.67	icsd_040850	MnO_6V_2	12.62
icsd_105220	NbRhSn	119.319	icsd_041802	Cl_3CrCs	12.62
icsd_107129	CoNbSb	119.319	icsd_043042	Cr_2FeSe_4	12.62
icsd_108317	CoSbZr	44.231	icsd_043412	Te_4Ti_3	12.58
icsd_190997	$MnSc_2Si$	160.67	icsd_052510	Te_4V_3	12.62
icsd_190999	$GeMnSc_2$	44.231	icsd_099989	Co_3Se_4	12.62
icsd_671364	BiMnPt	160.67	icsd_150462	MnO_2	12.62
icsd_028925	LaO_3V	166.101	icsd_169764	CrF_3K	12.62
icsd_028930	$CrLaO_3$	123.345	icsd_172782	$BrMnS_2Sb$	12.62
icsd_029118	$FeLaO_3$	166.101	icsd_188911	CoO_6V_2	12.62
icsd_076057	Mn_3NPd	166.101	icsd_193869	$Ni_{0.5}Se_2Ti$	12.62
icsd_422858	$CdCo_3N$	65.486	icsd_195677	$BiBrFeS_2$	12.58
icsd_052994	Co_2GeZn	166.1	icsd_281558	$IMnSbSe_2$	12.62
icsd_057985	$AlMnPt_2$	166.101	icsd_415138	$BiIMnSe_2$	12.62
icsd_191168	$GaMnPt_2$	166.101	icsd_415307	$BiBrMnS_2$	12.62
icsd_001143	$Cu_3O_8P_2$	2.4	icsd_601038	$CoCr_2Se_4$	12.62
icsd_024284	$B_2Co_2O_5$	2.6	icsd_625012	$CoSe_4V_2$	12.58
icsd_028151	CuO_6V_2	2.4	icsd_625931	Cr_2FeS_4	12.62
icsd_039439	$CuMoO_4$	2.6	icsd_626279	Cr_2MnS_4	12.58
icsd_039887	H_2CuO_5Se	2.4	icsd_626299	Cr_2MnSe_4	12.62
icsd_043508	AsFeS	2.6	icsd_626579	$CrRh_2Te_4$	12.62
icsd_050506	CuF_6Mo	2.4	icsd_626640	Cr_2S_4Ti	12.62
icsd_050507	CrF_6Mo	2.4	icsd_626896	Cr_2Te_4Ti	12.62
icsd_059720	$BiMnO_5V$	2.6	icsd_626901	Cr_2Te_4V	12.62
icsd_063057	$As_2Cu_3O_8$	2.4	icsd_633504	$FeSe_4Ti_2$	12.62
icsd_064660	CuF_6Pt	2.4	icsd_061078	$MnMoO_4$	13.67
icsd_068184	H_2CuO_5S	2.4	icsd_081060	$MoNiO_4$	13.67
icsd_087710	H_2FeO_5V	2.6	icsd_081061	$CoMoO_4$	13.68
icsd_095571	$LiMoS_2$	2.6	icsd_411172	$K_2Mn_3S_4$	13.67
icsd_099499	$C_6CuFeK_2N_6$	2.4	icsd_054919	$LaMnO_3$	14.79
icsd_100442	$As_2Fe_4O_{11}$	2.6	icsd_073900	LaO_3V	14.75
icsd_167202	$CoFLiO_4S$	2.4	icsd_079494	$IrLa_2NiO_6$	14.75
icsd_167608	$HFeLiO_5P$	2.4	icsd_079495	$CoIrLa_2O_6$	14.75
icsd_180390	$FFeO_4S$	2.4	icsd_088043	NiO_3Y	14.79
icsd_180391	$FLiNiO_4S$	2.4	icsd_089955	Ca_2FeMoO_6	14.75
icsd_184601	$FLiO_4PV$	2.4	icsd_092051	$LuNiO_3$	14.79
icsd_189335	MoO_6Sr_2Ti	2.4	icsd_092336	$CaFeO_3$	14.79
icsd_193472	$Cu_3Nb_2O_8$	2.4	icsd_095578	O_3VY	14.75
icsd_246513	$BaMn_2O_6Y$	2.4	icsd_096085	$CuGeO_3$	14.75
icsd_246811	$B_2Fe_2O_5$	2.6	icsd_096120	La_2NiO_6Ru	14.79
icsd_260257	$NiO_{10}Te_2V_2$	2.4	icsd_097744	$MnMoO_6Sr_2$	14.75
icsd_416823	$HCoO_5PZn$	2.4	icsd_151888	$Mn_{0.5}Ni_{0.5}O_3Y$	14.79
icsd_099699	$BaMn_2O_6Y$	3.3	icsd_152444	Ca_2NiO_6Os	14.79
icsd_036263	MoO_2	4.9	icsd_153857	Bi_2MnNiO_6	14.75
icsd_084868	$CaCuO_2$	4.7	icsd_163761	La_2MnO_6V	14.79
icsd_192247	CoY_3	4.9	icsd_181147	$FeMn_2O_6Sb$	14.79
icsd_021067	CuO_6V_2	5.13	icsd_186428	La_2MnNiO_6	14.79
icsd_046003	CoO_6V_2	5.15	icsd_188476	$Cr_{0.5}Mn_{0.5}O_3Y$	14.75
icsd_060512	DV_2	8.34	icsd_188982	$CoMnO_6Y_2$	14.75
icsd_069869	$CaClFeO_2$	8.32	icsd_191374	$CrMnO_6Y_2$	14.79
icsd_001503	O_2V	10.46	icsd_192122	$CoLa_2O_6Ti$	12.62
icsd_081569	$Fe_2O_{12}Se_4Sr$	10.42	icsd_192872	$MnNiO_6Y_2$	14.79
icsd_089471	O_2V	10.46	icsd_195628	$FeMn_2O_6Re$	14.75
icsd_100696	D_2FeTi	10.45	icsd_237528	In_2MnNiO_6	14.79
icsd_601978	H_2FeTi	10.45	icsd_238148	Ca_2FeO_6Os	14.75
icsd_000901	$AsClCu_2O_4$	11.54	icsd_251022	MnO_3Sc	14.75
icsd_000902	$AsClCo_2O_4$	11.5	icsd_251832	$MnNiO_6Sc_2$	14.79
icsd_051677	$H_3ClCu_2O_3$	11.54	icsd_252567	Mn_3O_6Re	14.79
icsd_065346	$ClFeLiMoO_4$	11.52	icsd_093795	$CoMoO_6Te$	18.19
icsd_162834	$BiFeO_3$	11.55	icsd_163978	$MnMoO_6Te$	18.19
icsd_240499	BrOTi	11.54	icsd_037026	$FeNaS_2$	23.51
icsd_415798	$Cl_2Co_2O_3Te$	11.5	icsd_015105	$LiMnO_2$	59.407
icsd_657748	O_2Ti	11.54	icsd_001898	NaO_5V_2	31.125
icsd_002225	Cl_3CrRb	12.62	icsd_042490	Cu_2GeMnS_4	31.127
icsd_015043	Fe_3Se_4	12.62	icsd_088640	LiO_5V_2	31.125
icsd_016722	Cr_3S_4	12.62	icsd_193986	Cu_2MnS_4Si	31.125
icsd_016884	Cr_2NiS_4	12.62	icsd_627355	Cu_2FeS_4Si	31.123
icsd_024566	S_4V_3	12.62	icsd_627741	$Cu_2GeMnSe_4$	31.127

TABLE S82. ICSD numbers, chemical formulas, and magnetic space groups (MSGs) for magnetic linear combinations of elementary band representation (LCEBR).

ICSD	Formula	MSG	ICSD	Formula	MSG
icsd_628396	Cu_2MnSe_4Si	31.127	icsd_090827	Cu_2FeS_4Sn	3.3
icsd_041646	$Ba_2Cu_3O_7Y$	47.253	icsd_027315	MoO_5V	85.62
icsd_081167	$Ba_2Cu_3LaO_7$	47.253	icsd_015451	Te_4Ti_5	87.78
icsd_161972	$Ba_2Cu_3LuO_7$	47.253	icsd_024563	S_4V_5	12.62
icsd_164175	$BaFe_2O_5Y$	51.291	icsd_042881	Te_4V_5	12.62
icsd_171434	$BaCo_2O_5Y$	51.296	icsd_055075	Se_4Ti_5	87.79
icsd_658677	Co_2InY	51.295	icsd_098191	$MoNiO_6Sr_2$	12.62
icsd_020933	Fe_2HfSi_2	57.38	icsd_150701	$FeMoO_6Sr_2$	12.62
icsd_087157	Fe_2ScSi_2	57.381	icsd_152440	NiO_6OsSr_2	12.62
icsd_033996	$CoCu_2O_3$	59.41	icsd_153544	$CoMoO_6Sr_2$	12.62
icsd_005432	CoMnSi	62.446	icsd_187669	$MnMoO_6Sr_2$	12.62
icsd_020461	BCoMo	62.443	icsd_191960	Ba_2CuO_6Os	12.62
icsd_041918	GeMnNi	62.447	icsd_192904	Ca_2MnO_6Ti	12.62
icsd_043896	AsCoRh	62.444	icsd_236435	CoO_6OsSr_2	12.62
icsd_044052	AsRhTi	62.445	icsd_245819	CuO_6OsSr_2	12.62
icsd_052968	CoGeMn	62.447	icsd_250818	$IrNiO_6Sr_2$	12.62
icsd_053283	CuGeTi	62.441	icsd_652166	Se_4V_5	12.62
icsd_067558	Cu_2NaO_2	62.444	icsd_067978	$BaCuFeO_5Y$	25.59
icsd_071221	Cu_2LiO_2	62.444	icsd_167073	F_6LiMnV	102.19
icsd_072411	CuMnP	62.443	icsd_202705	F_6Fe_2Li	34.158
icsd_072413	AsCuMn	62.444	icsd_291413	$MnMoO_6Te$	18.19
icsd_087197	CuSiTi	62.447	icsd_063423	$Ba_2Cu_3O_6Y$	115.285
icsd_098405	MoPRu	62.446	icsd_026721	Cu_2FeS_4Sn	42.221
icsd_107965	AsRhV	62.443	icsd_042489	Cu_2MnS_4Sn	121.331
icsd_151867	CrFeP	62.444	icsd_047165	Cu_2FeGeS_4	23.51
icsd_158732	MnO_3Ti	62.446	icsd_085126	Cu_2FeSe_4Sn	23.51
icsd_165243	FeNiSi	62.441	icsd_099292	$CoCu_2S_4Si$	23.51
icsd_165248	CoCrSi	62.449	icsd_099293	$CoCu_2GeS_4$	121.331
icsd_165254	NiSiV	62.449	icsd_099294	$CoCu_2S_4Sn$	121.331
icsd_165255	CrNiSi	62.446	icsd_099296	$CoCu_2Se_4Sn$	121.331
icsd_185418	MnO_3V	62.441	icsd_155904	Cu_2MnSe_4Sn	121.331
icsd_187466	O_3Ti_2	62.446	icsd_160047	$CuFe_2InSe_4$	121.327
icsd_246514	FeO_3Ti	62.445	icsd_627313	$Cu_2FeGeSe_4$	42.221
icsd_260758	Fe_3N	62.449	icsd_627368	Cu_2FeSe_4Si	23.51
icsd_610884	AsMnNi	62.446	icsd_015521	$ClFe_3O_8Pb_4$	65.486
icsd_611086	AsNiTi	62.443	icsd_098113	$Ba_2Cu_3LuO_6$	123.347
icsd_611097	AsNiV	62.443	icsd_187030	AlTi	53.334
icsd_614129	BFe_2Ni	62.446	icsd_004054	F_3KMn	55.358
icsd_622955	CoFeP	62.441	icsd_059553	In_4Ti_3	55.358
icsd_623660	CoGeV	62.444	icsd_042335	$AsCr_2$	67.503
icsd_624659	CoPV	62.449	icsd_044009	AsMnV	59.407
icsd_625259	Co_3Sn_2	62.447	icsd_049516	$ClFeMoO_4$	67.503
icsd_632538	FeMnP	62.449	icsd_084962	$CrCuO_3SSr_2$	59.407
icsd_632646	FeMoP	62.444	icsd_084963	$CuFeO_3SSr_2$	67.503
icsd_633116	FePV	62.443	icsd_088949	$BaMn_2O_5Y$	129.419
icsd_637435	GeNiV	62.444	icsd_169992	Ca_2CuFeO_3S	59.407
icsd_643093	MnNiP	62.449	icsd_169993	Ca_2CuFeO_3Se	59.407
icsd_646165	NiPTi	62.447	icsd_423230	AsCuMn	59.407
icsd_646176	NiPV	62.443	icsd_191628	La_2NiO_6Ti	71.536
icsd_670836	CFe_2Ti	62.444	icsd_670534	$CoFeLa_2O_6$	139.537
icsd_025761	$CAsV_3$	63.465	icsd_670535	$FeIrLa_2O_6$	139.537
icsd_079258	B_3V_2	63.465	icsd_200593	HNi_2	1.1
icsd_180767	Ni_3S_2	63.459	icsd_162263	Bi_2FeO_6Ti	1.1
icsd_189439	Fe_2O_3	63.464	icsd_246426	Bi_2CrFeO_6	146.1
icsd_246516	FeO_3Ti	63.459	icsd_191591	$CsFeMo_2O_8$	2.4
icsd_601350	B_3Cr_2	63.461	icsd_194588	$Ag_2FeO_8RbV_2$	2.4
icsd_610970	$AsNV_3$	63.459	icsd_194590	$Ag_2FeKO_8V_2$	2.4
icsd_617981	$CGeV_3$	63.459	icsd_245666	$FeMo_2O_8Rb$	2.4
icsd_618621	CPV_3	63.461	icsd_408193	$Ag_2BaMnO_8V_2$	2.4
icsd_634723	$GaNV_3$	63.461	icsd_417823	$C_6Mn_2N_6Ru$	147.15
icsd_637164	$GeNV_3$	63.465	icsd_417824	$C_6FeMn_2N_6$	147.15
icsd_644620	NPV_3	63.465	icsd_417825	$C_6Mn_2N_6Os$	147.15
icsd_050089	$Cu_6O_{10}Sr_4$	65.485	icsd_429825	$BaLi_2MnO_8V_2$	2.4
icsd_065881	$BaCu_3O_4$	65.485	icsd_015988	NiO_3Ti	2.6
icsd_044175	B_4Co_2Mo	71.535	icsd_016548	CoO_3Ti	2.4
icsd_188992	$GaMnNi_2$	71.536	icsd_024790	FeO_3Ti	2.6
icsd_416904	$Cu_3O_5Sr_2$	71.536	icsd_031853	$MnNiO_3$	2.4
icsd_670346	$CaMnO_3$	71.536	icsd_031854	$CoMnO_3$	148.19
icsd_036535	Cu_2O_2Tl	74.558	icsd_044407	MnO_3Ti	2.6
icsd_069870	Ca_2ClFeO_3	35.167	icsd_087943	F_3Ni	2.4

TABLE S83. ICSD numbers, chemical formulas, and magnetic space groups (MSGs) for magnetic linear combinations of elementary band representation (LCEBR).

ICSD	Formula	MSG	ICSD	Formula	MSG
icsd_201765	$CoLaO_3$	2.4	icsd_054259	NiSnTi	44.231
icsd_029133	CoF_3	5.13	icsd_054343	MnRhSb	44.231
icsd_029134	F_3Rh	5.15	icsd_076699	NiSbTi	119.319
icsd_626435	CrNiP	38.189	icsd_076702	NiSbV	44.231
icsd_201088	HNi_2	8.34	icsd_106680	FeSnTi	160.67
icsd_024796	$CrCuS_2$	8.34	icsd_107124	RuSbV	119.319
icsd_024798	$CrCuSe_2$	8.32	icsd_161715	GeMnNi	160.67
icsd_033995	$GaMo_4S_8$	8.32	icsd_182484	CrNiSb	44.231
icsd_036563	$GaMo_4Se_8$	8.32	icsd_184947	$GeMn_2$	160.67
icsd_036564	$AlMo_4S_8$	8.32	icsd_189702	$InTi_2$	44.231
icsd_158199	GaS_8V_4	8.32	icsd_191682	CoTeV	119.319
icsd_195253	$GaSe_8V_4$	8.32	icsd_191684	CoCrTe	119.319
icsd_039428	Cl_3Ti	15.87	icsd_191687	FeMnTe	44.231
icsd_031342	$Li_{0.33}S_2Ti$	12.62	icsd_670784	AlCrVZr	160.67
icsd_062661	$Mn_3Nb_6O_{11}$	12.58	icsd_670785	AlCrHfV	160.67
icsd_073874	Li_2NiO_2	165.96	icsd_670787	CrGaVZr	160.67
icsd_100782	$K_3O_8V_3$	12.62	icsd_670788	CrGaHfV	44.231
icsd_153864	$FeKMo_2O_8$	12.62	icsd_670790	CrInVZr	44.231
icsd_155025	$Fe_2In_2Se_5$	12.58	icsd_670791	CrHfInV	160.67
icsd_202907	$CsMo_2O_8V$	12.62	icsd_670792	CrScSiV	44.231
icsd_245665	$FeMo_2O_8Rb$	12.62	icsd_670793	CrGeScV	44.231
icsd_260887	$CsFeMo_2O_8$	12.58	icsd_670794	CrScSnV	160.67
icsd_429824	$BaLi_2MnO_8V_2$	12.58	icsd_670795	CrSiVY	160.67
icsd_429826	$BaCoNa_2O_8V_2$	12.58	icsd_670796	CrGeVY	44.231
icsd_429827	$BaFeNa_2O_8V_2$	12.62	icsd_670797	CrSnVY	44.231
icsd_024160	$CuFeO_2$	166.101	icsd_670798	CrKSV	160.67
icsd_026676	$CrCuO_2$	166.101	icsd_670799	CaCrPV	160.67
icsd_027803	$CoCuO_2$	12.58	icsd_670800	CrRbSV	44.231
icsd_031918	$CuFeO_2$	166.101	icsd_670801	CrPSrV	160.67
icsd_043740	NiO	12.58	icsd_671535	Mn_2Si	160.67
icsd_670109	$CoCuO_2$	12.62	icsd_051984	$InMnNi_2$	166.101
icsd_068847	FeS	36.176	icsd_053555	Fe_2SiV	166.101
icsd_042735	CoSiTi	189.223	icsd_053706	$GeMnRh_2$	166.101
icsd_042943	CoGeTi	38.191	icsd_057807	$AlFe_2Mo$	166.101
icsd_623085	CoGaHf	38.189	icsd_057976	$AlMnNi_2$	166.101
icsd_637069	GeMnRh	38.191	icsd_058071	$AlNi_2V$	166.101
icsd_648274	P_3V_5	63.461	icsd_076227	Mn_3Si	166.101
icsd_066546	$CuFeO_2$	194.268	icsd_102437	$CoGa_2Mn$	166.101
icsd_081489	$MnMoN_2$	63.457	icsd_102531	Co_2MnSn	166.101
icsd_082065	$CrCuO_2$	194.268	icsd_103803	$GaMnNi_2$	166.101
icsd_181348	AlN_3V_4	63.461	icsd_104936	$MnPbRh_2$	166.101
icsd_409451	CoCrGe	63.462	icsd_104964	$MnRh_2Sn$	166.101
icsd_624219	$CoMoP_2$	194.268	icsd_155336	$Ga_4Mn_4Ni_8$	166.101
icsd_629351	Cu_3Te_4V	111.255	icsd_186057	Fe_2GeTi	71.535
icsd_042978	CuMnSb	44.231	icsd_186061	Fe_2MnSi	166.101
icsd_053001	CoMnSb	160.67	icsd_187492	$FeGaNi_2$	71.536
icsd_053070	CoSbTi	44.231	icsd_188334	$GeMn_3$	166.101

V. ALTERMAGNETIC MATERIALS

Altermagnets constitute a novel magnetic class distinct from conventional antiferromagnets, attracting considerable interest due to their unique band characteristics and transport properties [22–24, 79, 80, 82–98].Altermagnets exhibit the collinear-compensated magnetic phase which are characterized by crystal-rotation symmetries connecting opposite-spin sublattices separated in the real space, i.e. the symmetry $[C_2||A]$, where C_2 is the 180° rotation of the spin space around an axis perpendicular to the spins, while transformations A that can be only real-space proper or improper rotations and cannot be real-space inversion. Based on this symmetry criterion, we identify 392 altermagnetic materials in our database, representing 13.5% of all compounds. A complete list of the candidate altermagnetic materials is provided in the Table S51. The magnetic structure, electronic band structures, and associated information of altermagnetic materials is available at `https://magdatabase.nju.edu.cn`, which is continuously updated. Below we present representative material of Altermagnetism CsV_2S_2O in section V A.

A. Representative Material of Altermagnetism CsV_2S_2O

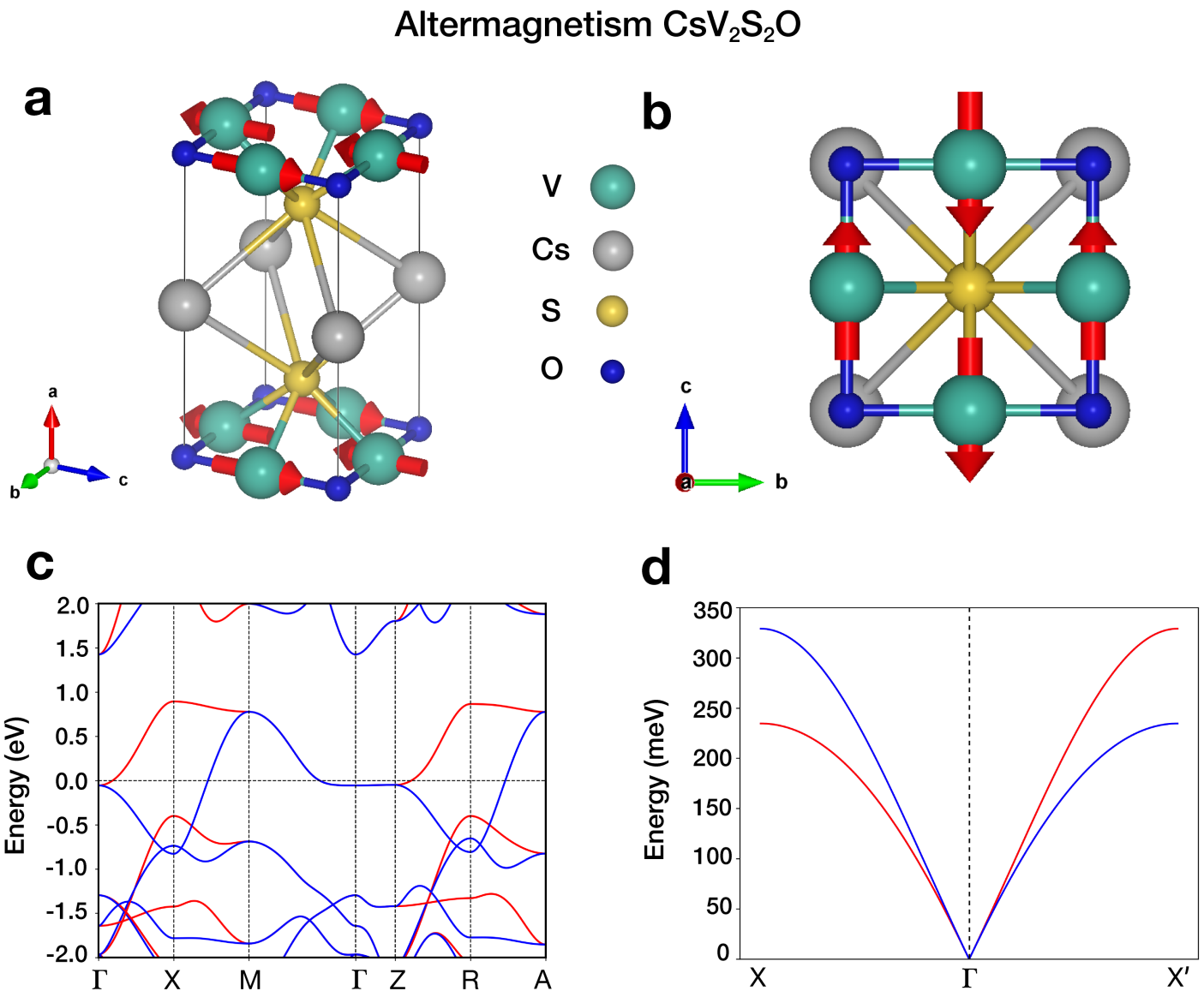


FIG. S6. (a)(b) Crystal structure of CsV_2S_2O. (c) Electron band splitting of CsV_2S_2O from first-principles calculations. (d) Chiral-magnon band splitting calculated based on the exchange interactions described in the main text, showing a maximum splitting of 94.4 meV at the X point.

CsV_2S_2O crystallizes in space group $P4/mmm$ (No. 123) with magnetic ions occupying the $1b$ Wyckoff positions, as shown in Fig. S6(a). It exhibits a pronounced altermagnetic spin splitting along high-symmetry paths [Fig. S6(b)], with a momentum-dependent maximum of about 1.7 eV near the X point, indicating a very strong electronic altermagnetic effect.

Typically, altermagnets exhibiting chiral splitting in magnon spectra originate from disparities in their exchange interactions with long-distance. In prototypical systems such as MnF_2 and MnTe, the exchange parameters (e.g., J_{7a} versus J_{7b} in MnF_2) produce minimal splitting amplitudes: experimental measurements show negligible chiral splitting in MnF_2 [99] and approximately 2 meV in MnTe [100]. Based on the magnetic force theorem and linear-response calculations [101–103], the nearest-neighbor exchange interaction is $J_1 = 56.4$ meV, while two symmetry-inequivalent next-nearest-neighbor interactions take values $J_{2a} = -2.3$ meV and $J_{2b} = -25.8$ meV. This large disparity reflects the nonequivalent magnetic environments of the two sublattices and gives rise to a sizable chiral-magnon band splitting. As shown in Fig. S6(c), the splitting reaches up to 94.4 meV at the high-symmetry X point in the Brillouin zone, an exceptionally large value among known materials.

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