

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

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I. DETAILED DESCRIPTION OF OUR STRATEGY BASED ON IRREDUCIBLE-REPRESENTATION BASIS-VECTOR, AND TAKE Mn_3GaN AS A DEMONSTRATIVE EXAMPLE

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 μ 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 $\mu = (m_{1x}, m_{1y}, m_{1z}, \dots, m_{Nx}, m_{Ny}, m_{Nz})$ span a representation Γ_{mag} of the parent space group, which is in general reducible and can be decomposed into irreducible representations as

$$\Gamma_{\text{mag}} = \sum_{\oplus i} n_i \Gamma_i(j). \quad (1)$$

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 μ 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,

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

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,

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

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 C_1 - C_{10} . The symmetry operations in C_1 - C_{10} are listed as follows:

$$\begin{aligned}
 C_1: & 1 \\
 C_3: & 2_{01\bar{1}}, 2_{011}, 2_{1\bar{1}0}, 2_{10\bar{1}}, 2_{101}, 2_{110} \\
 C_5: & 4_{001}^+, 4_{010}^-, 4_{010}^+, 4_{001}^-, 4_{100}^+, 4_{100}^- \\
 C_7: & m_{001}, m_{010}, m_{100} \\
 C_9: & 3_{11\bar{1}}^-, 3_{11\bar{1}}^-, 3_{11\bar{1}}^+, 3_{11\bar{1}}^+, 3_{11\bar{1}}^-, 3_{11\bar{1}}^+, 3_{11\bar{1}}^-, 3_{11\bar{1}}^+ \\
 C_2: & 2_{001}, 2_{010}, 2_{100} \\
 C_4: & 3_{11\bar{1}}^-, 3_{11\bar{1}}^-, 3_{11\bar{1}}^+, 3_{11\bar{1}}^+, 3_{11\bar{1}}^-, 3_{11\bar{1}}^+, 3_{11\bar{1}}^-, 3_{11\bar{1}}^+ \\
 C_6: & \bar{1} \\
 C_8: & m_{01\bar{1}}, m_{011}, m_{1\bar{1}0}, m_{10\bar{1}}, m_{101}, m_{110} \\
 C_{10}: & 4_{001}^+, 4_{010}^-, 4_{010}^+, 4_{001}^-, 4_{100}^+, 4_{100}^-
 \end{aligned}$$

	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 $R\bar{3}m'$, $R\bar{3}m$, $P4/mmm'$, $P4'/mmm'$, $Cmm'm'$, $C2'/m$, $C2/m$, $P2'/m$, 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 Γ_{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 $R\bar{3}m'$, $P4/mmm'$, and $Cmm'm'$ for the Γ_4^+ channel, and $R\bar{3}m$, $P4'/mmm'$, 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 $\{\phi_l^{(a)}\}$ 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

$$\begin{aligned}
 \phi_1^{(1)} &= (1, 0, 0; 1, 0, 0; 0, 0, 0), \\
 \phi_2^{(1)} &= (0, 1, 0; 0, 0, 0; 0, 1, 0), \\
 \phi_3^{(1)} &= (0, 0, 0; 0, 0, 1; 0, 0, 1),
 \end{aligned} \tag{4}$$

and

$$\begin{aligned}
 \phi_1^{(2)} &= (0, 0, 0; 0, 0, 0; 1, 0, 0), \\
 \phi_2^{(2)} &= (0, 0, 0; 0, 1, 0; 0, 0, 0), \\
 \phi_3^{(2)} &= (0, 0, 1; 0, 0, 0; 0, 0, 0).
 \end{aligned} \tag{5}$$

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 $R\bar{3}m'$, $P4/mmm'$, 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:

$$\eta^{(1)} \propto \phi_1^{(1)} + \phi_2^{(1)} + \phi_3^{(1)}, \quad \eta^{(2)} \propto \phi_1^{(2)} + \phi_2^{(2)} + \phi_3^{(2)}. \tag{6}$$

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,

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

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)–(7), the resulting magnetic moments on the three Mn ions of Mn_3GaN can be written as:

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

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 ($[\bar{1}11]$, $[1\bar{1}1]$, $[\bar{1}\bar{1}1]$, $[11\bar{1}]$), and twofold ($[\bar{1}\bar{1}0]$, $[110]$, $[01\bar{1}]$, $[0\bar{1}1]$, $[\bar{1}01]$, $[10\bar{1}]$) rotational axes, as well as in-plane directions perpendicular to the threefold axes ($[\bar{1}12]$, $[\bar{1}\bar{1}2]$, $[121]$, $[1\bar{2}1]$, $[12\bar{1}]$, $[\bar{1}2\bar{1}]$, $[211]$, $[2\bar{1}1]$, $[2\bar{1}\bar{1}]$, $[21\bar{1}]$) $[11]$.

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

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

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:

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

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.

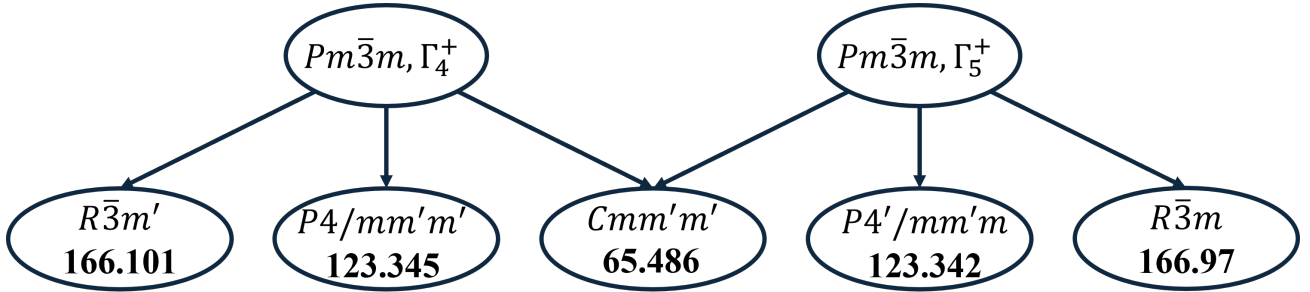


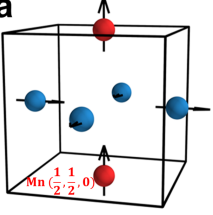
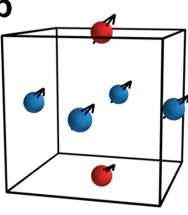
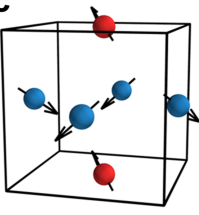
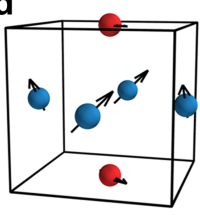
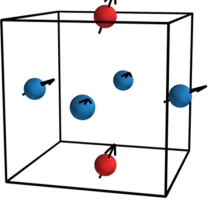
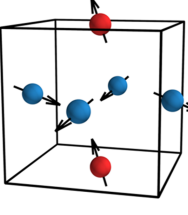
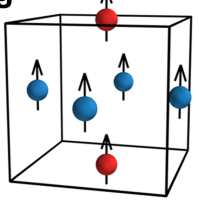
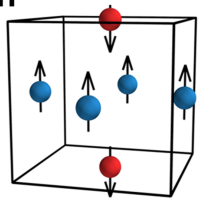
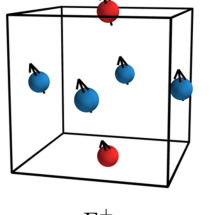
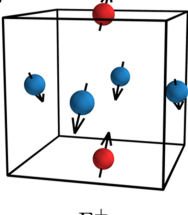
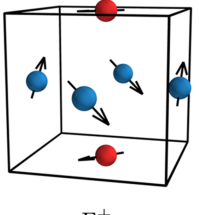
FIG. S1. **Symmetry-compatible MSGs for Mn_3GaN .** Maximal-symmetry candidate MSGs associated with the irreducible representations Γ_4^+ and Γ_5^+ .

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 Configuration	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]	$[\bar{1}\bar{1}\bar{1}]$	[110]
Magnetic Configuration	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 Configuration	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]	$[\bar{1}0\bar{1}]$	$[\bar{1}\bar{1}0]$	

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 [15].

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 [16]. 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 S3. 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 S4. 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 S5. 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 S6. 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 S7.

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

TABLE S3. 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 [15].

Materials	Crystallographic space group	Magnetic space group	Irreps
Fe ₄ O ₅ (0.999) [17]	<i>Cmcm</i> (No.63)	<i>Cm'</i> <i>c</i> 2 ₁ ' (No.36.174)	Γ_3^-, Γ_4^+
Fe ₄ O ₅ (0.1000) [17]	<i>Cmcm</i> (No.63)	<i>P</i> 2 ₁ ' (No.4.9)	$\Gamma_3^-, \Gamma_4^+, \Gamma_3^+$
BaFe ₂ Se ₄ (0.1024)[18]	<i>I4/m</i> (No.87)	<i>C</i> 2' (No.5.15)	$\Gamma_3^+, \Gamma_4^+, \Gamma_3^-, \Gamma_4^-$
Mn ₃ Si ₂ Te ₆ (0.1026)[19]	<i>P</i> 31 <i>c</i> (No.163)	<i>C</i> 2'/ <i>c</i> ' (No.15.89)	Γ_3^+, Γ_2^+
LuFe ₄ Ge ₂ (0.140)[20]	<i>P</i> 4 ₂ / <i>mmn</i> (No.136)	<i>Pn'</i> <i>n'</i> <i>m'</i> (No.58.399)	Γ_2^-, Γ_2^+
LiFePO ₄ (0.152)[21]	<i>Pnma</i> (No.62)	<i>P</i> 2 ₁ / <i>c</i> ' (No.14.78)	Γ_2^-, Γ_1^-
CaMnGe ₂ O ₆ (0.155) [22]	<i>C</i> 2/ <i>c</i> (No.15)	<i>P</i> 1' (No.2.6)	Γ_2^-, Γ_1^-
SrMn(VO ₄)(OH) (0.165)[23]	<i>P</i> 2 ₁ 2 ₁ 2 ₁ (No.19)	<i>P</i> 2 ₁ (No.4.7)	Γ_1, Γ_3
FePO ₄ (0.17) [24]	<i>Pnma</i> (No.62)	<i>P</i> 2 ₁ 2 ₁ 2 ₁ (No.19.25)	Γ_1^-, Γ_1^+
Co ₄ Nb ₂ O ₉ (0.196) [25]	<i>P</i> 3 <i>c</i> 1 (No.165)	<i>C</i> 2'/ <i>c</i> ' (No.15.88)	Γ_3^-, Γ_1^-
Mn ₃ Ge (0.203)[26]	<i>P</i> 6 ₃ / <i>mmc</i> (No.194)	<i>C</i> 2'/ <i>m'</i> (No.12.62)	Γ_6^+, Γ_2^+
RbMnF ₄ (0.329)[27]	<i>P</i> 2 ₁ / <i>a</i> (No.14)	<i>P</i> 1' (No.2.4)	Γ_1^+, Γ_2^+
LiCoPO ₄ (0.384)[28]	<i>Pnma</i> (No.62)	<i>P</i> 2 ₁ '/ <i>c</i> (No.14.77)	Γ_2^-, Γ_4^-
LiCoPO ₄ (0.385)[29]	<i>Pnma</i> (No.62)	<i>P</i> 2 ₁ / <i>c</i> ' (No.14.78)	Γ_2^-, Γ_1^-
YMnO ₃ (0.44)[30]	<i>P</i> 6 ₃ <i>cm</i> (No.185)	<i>P</i> 6 ₃ ' (No.173.131)	Γ_3, Γ_4
La ₂ NiO ₄ (0.45)[31]	<i>P</i> 4 ₂ / <i>ncm</i> (No.138)	<i>Pc'</i> <i>c'</i> <i>n</i> (No.56.369)	Γ_3^+, Γ_4^+
Cr ₂ S ₃ (0.5)[32]	<i>R</i> 3 (No.148)	<i>P</i> 1' (No.2.4)	$\Gamma_2^+, \Gamma_3^+, \Gamma_1^+$
NaCrSi ₂ O ₆ (0.504)[33]	<i>C</i> 2/ <i>c</i> (No.15)	<i>P</i> 1' (No.2.6)	Γ_1^-, Γ_2^-
CaMn ₂ Sb ₂ (0.523)[34]	<i>P</i> 3 <i>m</i> 1 (No.164)	<i>P</i> 1' (No.2.6)	Γ_3^-, Γ_1^-
CaMnGe (0.601)[35]	<i>P</i> 4/ <i>nmn</i> (No.129)	<i>P</i> 2 ₁ / <i>m'</i> (No.11.53)	Γ_2^-, Γ_5^-
CaMnGe (0.602)[35]	<i>P</i> 4/ <i>nmn</i> (No.129)	<i>P</i> 2 ₁ / <i>m'</i> (No.11.53)	Γ_2^-, Γ_5^-
Mn ₃ Ga (0.641)[36]	<i>I</i> 4/ <i>mmm</i> (No.139)	<i>C</i> 2'/ <i>m'</i> (No.12.62)	Γ_3^+, Γ_5^+
YVO ₃ (0.788)[37]	<i>P</i> 2 ₁ / <i>b</i> 11 (No.14)	<i>P</i> 1' (No.2.4)	Γ_1^+, Γ_2^+
NbMnP (0.803) [38]	<i>Pnma</i> (No.62)	<i>Pm'</i> <i>n</i> 2 ₁ ' (No.31.125)	Γ_3^+, Γ_4^-
Fe ₂ WO ₆ (0.812) [39]	<i>Pbcn</i> (No.60)	<i>Pn'</i> <i>c</i> 2' (No.30.113)	Γ_3^+, Γ_2^-
FeSb ₂ O ₄ (0.97) [40]	<i>P</i> 4 ₂ / <i>mbc</i> (No.135)	<i>Pmc</i> 2 ₁ (No.26.66)	Γ_2^+, Γ_5^-

TABLE S4. 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 [15].

Materials			
AlFe ₂ B ₂ (0.414)	Ba ₂ Mn ₃ Sb ₂ O ₂ (0.471)	Ba ₂ MnSi ₂ O ₇ (0.229)	BaCr ₂ As ₂ (0.365)
BaMn ₂ As ₂ (0.18)	BaMn ₂ Bi ₂ (0.89)	BaMn ₂ Ge ₂ (0.605)	BaMn ₂ Ge ₂ (0.606)
BaMn ₂ P ₂ (0.464)	BaMn ₂ Sb ₂ (0.470)	BaMnSb ₂ (0.611)	Bi ₂ CuO ₄ (0.348)
Bi ₂ CuO ₄ (0.694)	CaMn ₂ Ge ₂ (0.603)	CaMn ₂ Ge ₂ (0.604)	CaMnBi ₂ (0.72)
CaMnSi (0.599)	CaMnSi (0.600)	CoF ₂ (0.178)	CoF ₃ (0.334)
CoTa ₄ Se ₈ (0.1036)	Cr ₂ O ₃ (0.59)	CrNb ₄ S ₈ (0.708)	CrSb (0.528)
Fe ₂ TeO ₆ (0.142)	Fe ₂ TeO 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 ₂ O ₃ Mn ₂ Se ₂ (0.1091)	La ₂ O ₃ Mn ₂ Se ₂ (0.1092)	La ₂ O ₃ Mn ₂ Se ₂ (0.1093)
LaBaMn ₂ O ₆ (0.737)	LaBaMn ₂ O ₆ (0.738)	LaCrO ₃ (0.416)	LaMn ₂ Si ₂ (0.472)
LaMn ₂ Si 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 ₂ F 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 ₂ Mn ₃ As ₂ O ₂ (0.212)	Sr ₄ Fe ₄ O ₁₁ (0.401)	SrCr ₂ As ₂ (0.364)
SrMnBi ₂ (0.73)	SrMnSb ₂ (0.767)	YMnO ₃ (0.6)	[Na(OH) ₂] ₃ Mn(NCS) ₃ (0.1078)

TABLE S5. 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 [15].

Materials				
CaMn ₂ Sb ₂ (0.92)	Mn ₂ Au (0.1081)	Mn ₂ Au (0.639)	Mn ₂ Au (0.640)	
Mn ₃ GaN (0.177)	Mn ₃ ZnN (0.273)	MnNb ₄ S ₈ (0.709)	MnPtGa (0.395)	
MnTa ₄ S ₈ (0.711)	MnTe (0.800)	SrMn ₂ As ₂ (0.482)	VNb ₃ S ₆ (0.712)	

TABLE S6. Table of 49 materials cannot be described by our method due to deviations of magnetic moments from high-symmetry directions, corresponding 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 [15].

Materials				
Ag ₂ RuO ₄ (0.918)	BaFe ₂ Se ₂ O (0.988)	BaMnFeF ₇ (0.577)	Ca ₂ MnReO ₆ (0.204)	Ca ₂ RuO ₄ (0.398)
CaFe ₅ O ₇ (0.357)	Co ₂ SiO ₄ (0.218)	Co ₂ SiO ₄ (0.219)	Co ₄ Nb ₂ O ₉ (0.197)	Co ₄ Nb ₂ O ₉ (0.529)
Co ₄ Ta ₂ O ₉ (0.511)	CoFePO ₅ (0.262)	CoSO ₄ (0.571)	CoSO ₄ (0.96)	CoSe ₂ O ₅ (0.119)
Cr ₂ F ₅ (0.576)	Cs ₂ Cu ₃ SnF ₁₂ (0.506)	CsMn ₂ F ₆ (0.726)	Cu ₂ (OD) ₃ Cl (0.295)	Cu ₂ OSO ₄ (0.612)
Fe(N(CN ₂)) ₂ (0.132)	Fe ₂ SeO (0.1061)	Fe ₂ SiO ₄ (0.1072)	Fe ₂ SiO ₄ (0.221)	Fe ₂ WO ₆ (0.809)
Fe ₂ WO ₆ (0.810)	GaV ₄ S ₈ (0.756)	KMnF ₄ (0.328)	La ₂ CoIrO ₆ (0.375)	LiNiPO ₄ (0.88)
Mn ₂ GeO ₄ (0.101)	Mn ₂ GeO ₄ (0.102)	Mn ₂ SiO ₄ (0.220)	Mn ₃ CoGe (0.900)	Mn ₃ IrGe (0.899)
Mn ₃ IrSi (0.898)	Mn ₃ RhGe (0.1005)	Mn ₃ Sn ₂ (0.663)	MnNb ₂ O ₆ (0.819)	MnPtGa (0.396)
MnTa ₂ O ₆ (0.818)	MnV ₂ O ₄ (0.64)	RbRuO ₄ (0.924)	SrCo(VO ₄)(OH) (0.287)	SrFe ₂ S ₂ O (0.762)
SrFe ₂ Se ₂ O (0.761)	Y ₂ MnCoO ₆ (0.164)	YFe ₄ Ge ₂ (0.27)	ZrCo ₂ Ge ₄ O ₁₂ (0.314)	

TABLE S7. 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 [15].

Materials				
Ba ₂ CoGe ₂ O ₇ (0.56)	Ba ₃ NiRu ₂ O ₉ (0.748)	BaCrF ₅ (0.303)	BaCuF ₄ (0.191)	BaFe ₂ S ₂ O (0.987)
BaNi ₂ P ₂ O ₈ (0.215)	Bi ₂ CuO ₄ (0.695)	BiCrO ₃ (0.138)	Ca ₂ Fe ₂ O ₅ (0.1080)	Ca ₂ FeOsO ₆ (0.682)
Ca ₂ MnGaO ₅ (0.825)	Ca ₂ NiOsO ₆ (0.796)	CaCu ₃ Fe ₂ Sb ₂ O ₁₂ (0.672)	CaFe ₂ O ₄ (0.968)	CaFe ₂ O ₄ (0.969)
CaFe ₄ Al ₈ (0.236)	CaFe ₅ O ₇ (0.358)	CaIrO ₃ (0.79)	CaMnGe ₂ O ₆ (0.156)	Co ₂ Mo ₃ O ₈ (0.332)
Co ₂ Mo ₃ O ₈ (0.338)	Co ₃ Sn ₂ S ₂ (0.860)	Co ₃ Sn ₂ S ₂ (0.861)	Co ₄ Nb ₂ O ₉ (0.111)	CoCO ₃ (0.114)
CoSe ₂ O ₅ (0.161)	Cr ₂ CoAl (0.1073)	Cr ₂ MoO ₆ (0.1023)	Cr ₂ O ₃ (0.110)	Cr ₂ TeO ₆ (0.143)
Cr ₂ TeO ₆ (0.76)	Cr ₂ TeO ₆ (0.959)	Cr ₂ WO ₆ (0.144)	Cr ₂ WO 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 ₂ Mo ₃ O ₈ (0.331)	Fe ₂ O ₃ (0.299)	Fe ₂ O ₃ (0.300)	Fe ₂ O ₃ -alpha (0.65)	Fe ₂ PO ₅ (0.263)
Fe ₂ SiO ₄ (0.1071)	Fe ₂ WO ₆ (0.811)	Fe ₂ WO ₆ (0.813)	Fe ₂ WO ₆ (0.814)	Fe ₃ (PO ₄) ₂ (0.264)
Fe ₃ (PO ₄) ₂ (OH) ₂ (0.392)	Fe ₃ F ₈ (H ₂ O) ₂ (0.582)	Fe ₄ Nb ₂ O ₉ (0.441)	Fe ₄ Nb ₂ O ₉ (0.443)	FeBO ₃ (0.112)
FeF ₃ (0.335)	FeF ₃ (0.581)	FeOHSO ₄ (0.760)	FeOOH (0.399)	FeSO ₄ F (0.128)
GaFeO ₃ (0.38)	InCrO ₃ (0.308)	K ₂ ReI ₆ (0.434)	K ₂ ReI ₆ (0.553)	KFeS ₂ (0.633)
KMnF ₃ (0.432)	La ₂ LiRuO ₆ (0.148)	LaBaMn ₂ O ₅ (0.735)	LaCrO ₃ (0.323)	LaCrO ₃ (0.417)
LaMnO ₃ (0.1)	LaMnO ₃ (0.642)	Li ₂ Co(SO ₄) ₂ (0.121)	Li ₂ Mn(SO ₄) ₂ (0.122)	Li ₂ Ni(SO ₄) ₂ (0.714)
LiCrGe ₂ O ₆ (0.217)	LiCrGe ₂ O ₆ (0.961)	LiCrGe ₂ O ₆ (0.962)	LiCrGe ₂ O ₆ (0.963)	LiCrGe ₂ O ₆ (0.964)
LiFeP ₂ O ₇ (0.83)	LiFeSi ₂ O ₆ (0.28)	LiMn ₆ Sn 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 ₂ FeReO ₆ (0.541)	Mn ₂ Mo ₃ O ₈ (0.333)	Mn ₂ Sb (0.855)	Mn ₂ SeO ₃ F ₂ (0.755)	Mn ₃ AlN (0.275)
Mn ₃ AlN (0.276)	Mn ₃ As ₂ (0.512)	Mn ₃ As (0.279)	Mn ₃ As (0.280)	Mn ₃ Ge (0.377)
Mn ₃ Ir (0.108)	Mn ₃ IrGe (0.1006)	Mn ₃ Pt (0.109)	Mn ₃ Sn (0.199)	Mn ₃ Sn (0.200)
Mn ₃ Sn ₂ (0.662)	Mn ₃ Ti ₂ Te ₆ (0.176)	Mn ₄ N (0.274)	Mn ₄ Nb ₂ O ₉ (0.507)	Mn ₄ Ta ₂ O ₉ (0.477)
Mn ₄ Ta ₂ O ₉ (0.526)	Mn ₅ Ge ₃ (0.286)	MnCO ₃ (0.115)	MnCoGe (0.445)	MnGeN ₂ (0.1065)
MnGeO ₃ (0.312)	MnLaMnSbO ₆ (0.234)	MnNb ₂ O ₆ (0.815)	MnPS ₃ (0.163)	MnPS ₃ (0.180)
MnPS ₃ (0.524)	MnPd ₂ (0.798)	MnSiN ₂ (0.1066)	MnTa ₂ O ₆ (0.816)	MnTiO ₃ (0.19)
MnTiO ₃ (0.50)	Na ₂ BaCo(VO ₄) ₂ (0.266)	NaCrGe ₂ O ₆ (0.297)	NaMnFeF ₆ (0.310)	NaOsO ₃ (0.25)
NiCO ₃ (0.113)	NiCr ₂ O ₄ (0.4)	NiCr ₂ O ₄ (0.895)	NiF ₂ (0.36)	NiFePO ₅ (0.261)
RbFe ₂ F ₆ (0.192)	RbFeS ₂ (0.636)	ScCrO ₃ (0.307)	ScMnO ₃ (0.7)	Sr ₂ CoOsO ₆ (0.210)
Sr ₂ CoTeO ₆ (0.301)	Sr ₂ CoTeO ₆ (0.937)	Sr ₂ Fe ₂ O ₅ (0.1084)	Sr ₂ LuRuO ₆ (0.420)	Sr ₂ MnGaO ₅ (0.823)
Sr ₂ MnTeO ₆ (0.936)	Sr ₂ NiTeO ₆ (0.934)	Sr ₂ ScOsO ₆ (0.917)	Sr ₂ YRuO ₆ (0.795)	Sr ₄ Fe ₄ O ₁₁ (0.402)
SrMnO ₃ (0.1018)	SrMnO ₃ (0.1019)	SrRuO ₃ (0.732)	Tl ₃ Fe ₂ S ₄ (0.801)	TiCrO ₃ (0.309)
V ₂ WO ₆ (0.966)	Y ₂ Cu ₂ O ₅ (0.241)	YBaMn ₂ O ₅ (0.739)	YCo ₃ (0.859)	YCrO ₃ (0.586)
YCrO ₃ (0.947)	YNi ₄ Si (0.374)	YRuO ₃ (0.513)	YVO ₃ (0.787)	ZrMn ₂ Ge ₄ O 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 S8.

TABLE S8. 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[15].

	Materials				
Our framework successfully predict the experimental magnetic ground states for these materials	AlFe ₂ B ₂ (0.414)	Ba ₂ CoGe ₂ O ₇ (0.56)	Ba ₂ MnSi ₂ O ₇ (0.229)	Ba ₃ NiRu ₂ O ₉ (0.748)	BaCr ₂ As ₂ (0.365)
	BaCrF ₅ (0.303)	BaCuF ₄ (0.191)	BaFe ₂ S ₂ O (0.987)	BaMn ₂ As ₂ (0.18)	BaMn ₂ Bi ₂ (0.89)
	BaMn ₂ Ge ₂ (0.605)	BaMn ₂ Ge ₂ (0.606)	BaMn ₂ P ₂ (0.464)	BaMn ₂ Sb ₂ (0.470)	BaMnSb ₂ (0.611)
	BaNi ₂ P ₂ O ₈ (0.215)	Bi ₂ CuO ₄ (0.348)	Bi ₂ CuO ₄ (0.694)	Bi ₂ CuO ₄ (0.695)	BiCrO ₃ (0.138)
	Ca ₂ Fe ₂ O ₅ (0.1080)	Ca ₂ FeOsO ₆ (0.682)	Ca ₂ NiOsO ₆ (0.796)	CaCu ₃ Fe ₂ Sb ₂ O ₁₂ (0.672)	CaFe ₅ O ₇ (0.358)
	CaIrO ₃ (0.79)	CaMn ₂ Ge ₂ (0.603)	CaMn ₂ Ge ₂ (0.604)	CaMn ₂ Sb ₂ (0.92)	CaMnBi ₂ (0.72)
	CaMnGe ₂ O ₆ (0.156)	CaMnSi (0.599)	CaMnSi (0.600)	Co ₂ Mo ₃ O ₈ (0.332)	Co ₂ Mo ₃ O ₈ (0.338)
	Co ₃ Sn ₂ S ₂ (0.860)	Co ₃ Sn ₂ S ₂ (0.861)	Co ₄ Nb ₂ O ₉ (0.111)	CoCO ₃ (0.114)	CoF ₂ (0.178)
	CoF ₃ (0.334)	CoSe ₂ O ₅ (0.161)	CoTa ₄ Se ₈ (0.1036)	Cr ₂ O ₃ (0.110)	Cr ₂ O ₃ (0.59)
	Cr ₂ TeO ₆ (0.143)	Cr ₂ TeO ₆ (0.76)	Cr ₂ TeO ₆ (0.959)	Cr ₂ WO ₆ (0.144)	Cr ₂ WO 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 ₂ Mo ₃ O ₈ (0.331)	Fe ₂ O ₃ -alpha (0.65)	Fe ₂ PO ₅ (0.263)	Fe ₂ SiO ₄ (0.1071)
	Fe ₂ TeO ₆ (0.142)	Fe ₂ TeO ₆ (0.960)	Fe ₂ WO ₆ (0.814)	Fe ₃ (PO ₄) ₂ (OH) ₂ (0.392)	Fe ₃ F ₈ (H ₂ O) ₂ (0.582)
	FeBO ₃ (0.112)	FeCO ₃ (0.116)	FeF ₃ (0.335)	FeF ₃ (0.581)	FeHSO ₄ (0.760)
	FeOOH (0.399)	FeSO ₄ F (0.128)	GaFeO ₃ (0.38)	InCrO ₃ (0.308)	K ₂ ReI ₆ (0.434)
	K ₂ ReI 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 ₂ LiRuO ₆ (0.148)
	La ₂ O ₃ Mn ₂ Se ₂ (0.1092)	La ₂ O ₃ Mn ₂ Se ₂ (0.1093)	LaBaMn ₂ O ₆ (0.737)	LaBaMn ₂ O ₆ (0.738)	LaCrO ₃ (0.323)
	LaCrO ₃ (0.416)	LaCrO ₃ (0.417)	LaMn ₂ Si ₂ (0.472)	LaMn ₂ Si ₂ (0.498)	LaMnAsO (0.619)
	LaMnAsO (0.624)	LaMnSbO (0.667)	Li ₂ Co(SO ₄) ₂ (0.121)	Li ₂ Mn(SO ₄) ₂ (0.122)	Li ₂ Ni(SO ₄) ₂ (0.714)
	LiCoPO ₄ (0.193)	LiCoPO ₄ (0.383)	LiFe ₂ F ₆ (0.501)	LiFe ₂ P ₂ O ₇ (0.83)	LiFePO ₄ (0.95)
	LiMn ₆ Sn 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 ₂ Au (0.1081)	Mn ₂ Au (0.639)	Mn ₂ Au (0.640)	Mn ₂ FeO ₆ (0.541)
	Mn ₂ Sb (0.855)	Mn ₃ As ₂ (0.512)	Mn ₃ GaN (0.177)	Mn ₃ Ge (0.377)	Mn ₃ Ir (0.108)
	Mn ₃ Sn (0.199)	Mn ₃ Sn (0.200)	Mn ₃ Ti ₂ Te ₆ (0.176)	Mn ₃ ZnN (0.273)	Mn ₄ N (0.274)
	Mn ₄ Nb ₂ O ₉ (0.507)	Mn ₄ Ta ₂ O ₉ (0.477)	Mn ₄ Ta ₂ O ₉ (0.526)	Mn ₅ Ge 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 ₂ O ₆ (0.815)	MnNb ₄ S ₈ (0.709)	MnPS ₃ (0.163)	MnPS ₃ (0.180)	MnPS ₃ (0.524)
	MnPd ₂ (0.798)	MnSiN ₂ (0.1066)	MnTa ₂ O ₆ (0.816)	MnTa ₄ S ₈ (0.711)	MnTe (0.800)
	MnTe ₂ (0.20)	MnTiO ₃ (0.19)	MnTiO ₃ (0.50)	Na ₂ BaCo(VO ₄) ₂ (0.266)	NaCrGe ₂ O 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 ₂ O ₄ (0.4)	NiCrO ₄ (0.896)	NiF ₂ (0.36)
	NiFePO ₅ (0.261)	NiS ₂ (0.150)	PbNiO ₃ (0.21)	RbFe ₂ F ₆ (0.192)	RbFeS ₂ (0.636)
	RbFeSe ₂ (0.638)	RuO ₂ (0.607)	ScCrO ₃ (0.307)	Sr ₂ CoTeO ₆ (0.301)	Sr ₂ CoTeO ₆ (0.937)
	Sr ₂ LuRuO ₆ (0.420)	Sr ₂ MnGaO ₅ (0.823)	Sr ₂ MnTeO ₆ (0.936)	Sr ₂ NiTeO ₆ (0.934)	Sr ₂ ScOsO ₆ (0.917)
	Sr ₂ YRuO ₆ (0.795)	Sr ₄ Fe ₄ O ₁₁ (0.401)	Sr ₄ Fe ₄ O ₁₁ (0.402)	SrCr ₂ As ₂ (0.364)	SrMn ₂ As ₂ (0.482)
	SrMnBi ₂ (0.73)	SrMnO ₃ (0.1018)	SrMnO ₃ (0.1019)	SrRuO ₃ (0.732)	TlCrO ₃ (0.309)
	V ₂ WO ₆ (0.966)	VNb ₃ S ₆ (0.712)	Y ₂ Cu ₂ O ₅ (0.241)	YCrO ₃ (0.586)	YCrO ₃ (0.947)
	YVO ₃ (0.787)	ZrMn ₂ Ge ₄ O ₁₂ (0.315)	[Na(OH) ₂] ₃ Mn(NCS) ₃ (0.1078)		
Our framework failed to identify the experimental magnetic ground state for these materials	Ba ₂ Mn ₃ Sb ₂ O ₂ (0.471)	Ca ₂ MnGaO ₅ (0.825)	CaFe ₂ O ₄ (0.968)	CaFe ₂ O ₄ (0.969)	CaFe ₄ Al ₈ (0.236)
	Cr ₂ CoAl (0.1073)	Cr ₂ MoO ₆ (0.1023)	CrNb ₄ S ₈ (0.708)	CsMnF ₄ (0.327)	Fe ₂ O ₃ (0.299)
	Fe ₂ O ₃ (0.300)	Fe ₂ WO ₆ (0.811)	Fe ₂ WO ₆ (0.813)	Fe ₃ (PO ₄) ₂ (0.264)	Fe ₄ Nb ₂ O ₉ (0.441)
	Fe ₄ Nb ₂ O ₉ (0.443)	La ₂ O ₃ Mn ₂ Se ₂ (0.1091)	LaBaMn ₂ O ₅ (0.735)	LaMnO ₃ (0.1)	LaMnO ₃ (0.642)
	LaMnSi ₂ (0.778)	LaMnSi ₂ (0.779)	LaMnSi ₂ (0.780)	LiCrGe ₂ O ₆ (0.217)	LiCrGe ₂ O ₆ (0.961)
	LiCrGe ₂ O ₆ (0.962)	LiCrGe ₂ O ₆ (0.963)	LiCrGe ₂ O ₆ (0.964)	LiFe ₂ O ₆ (0.28)	LuFeO ₃ (0.117)
	LuVO ₃ (0.984)	MgMnO ₃ (0.277)	Mn ₂ Mo ₃ O ₈ (0.333)	Mn ₂ SeO ₃ F ₂ (0.755)	Mn ₃ AlN (0.275)
	Mn ₃ AlN (0.276)	Mn ₃ As (0.279)	Mn ₃ As (0.280)	Mn ₃ IrGe (0.1006)	Mn ₃ Pt (0.109)
	Mn ₃ Sn ₂ (0.662)	MnCoGe (0.445)	MnPtGa (0.395)	NiCr ₂ O ₄ (0.895)	ScMnO ₃ (0.7)
	Sr ₂ CoOsO ₆ (0.210)	Sr ₂ Fe ₂ O ₅ (0.1084)	Sr ₂ Mn ₃ As ₂ O ₂ (0.212)	SrMnSb ₂ (0.767)	Tl ₃ Fe ₂ S ₄ (0.801)
	YBaMn ₂ O ₅ (0.739)	YCo ₃ (0.859)	YMnO ₃ (0.6)	YNi ₄ Si (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) [41]. 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 [16]. 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 S9-S31, S32-S35, S36-S37, S38-S47, S48-S49, S50-S56, respectively.

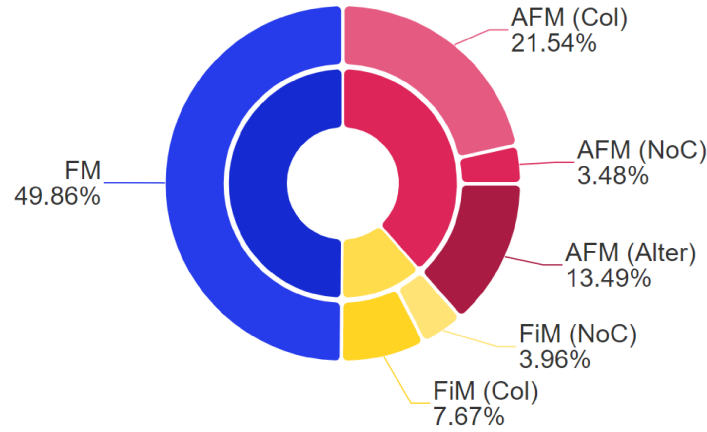


FIG. S2. **Magnetic and topological classification of our magnetic structure database.** (a) Statistics of magnetic ground-state classification. Among the 2,906 identified magnetic materials, 49.86% exhibit ferromagnetic (FM) ordering, 11.63% are ferrimagnetic (FiM), and the remaining 38.51% are antiferromagnetic (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 S9-S31, including their chemical formula, space group, magnetic space group, band gap and corresponding irreducible representations of crystallographic space group.

TABLE S9. 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 ₂ F ₁₂	2	2.4	0.80	Γ_1^+
icsd_065186	AgF ₁₂ Sb ₂	2	2.4	0.90	Γ_1^+
icsd_051505	AgF ₆ Sn	2	2.4	0.71	Γ_1^+
icsd_051506	AgF ₆ Ti	2	2.4	0.11	Γ_1^+
icsd_063058	As ₂ CuNa ₄ O ₈	2	2.4	2.41	Γ_1^+
icsd_018115	As ₂ CuO ₈ Zn ₂	2	2.4	2.17	Γ_1^+
icsd_062544	AuCuF ₅	2	2.4	1.89	Γ_1^+
icsd_174291	Ba ₂ BiIrO ₆	2	2.4	0.40	Γ_1^+
icsd_174140	Ba ₂ IrLaO ₆	2	2.4	0.33	Γ_1^+
icsd_037027	Ba ₂ LaO ₆ Ru	2	2.4	1.19	Γ_1^+
icsd_246513	BaMn ₂ O ₆ Y	2	2.4	0.00	Γ_1^+
icsd_424465	Br ₁₀ CoY ₆	2	2.4	0.01	Γ_1^+
icsd_423462	Br ₅ W	2	2.4	0.25	Γ_1^+
icsd_172335	C ₂ CuF ₆ O ₆ S ₂	2	2.4	2.19	Γ_1^+
icsd_099499	C ₆ CuFeK ₂ N ₆	2	2.4	1.11	Γ_1^+
icsd_171007	Ca ₂ Cl ₂ CuO ₁₀ Te ₄	2	2.4	2.06	Γ_1^+
icsd_249777	Cd ₂ CuO ₈ P 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 ₄ W ₂	2	2.4	0.08	Γ_1^+
icsd_084620	Cl ₅ Mo	2	2.4	0.43	Γ_1^+
icsd_078789	Cl ₆ ISe ₆ W	2	2.4	0.36	Γ_1^+
icsd_415768	Cl ₈ NW ₂	2	2.4	0.43	Γ_1^+
icsd_099580	Co ₂ Na ₆ O ₆	2	2.4	1.98	Γ_1^+
icsd_424841	Co ₁₀ Y ₆	2	2.4	0.00	Γ_1^+
icsd_092852	CoLi ₂ O ₈ W ₂	2	2.4	2.92	Γ_1^+
icsd_062676	CrNa ₄ O ₄	2	2.4	1.16	Γ_1^+
icsd_050444	Cs ₄ CuO ₇ Si ₂	2	2.4	2.02	Γ_1^+
icsd_409506	Cs ₆ NiO ₈ Si ₂	2	2.4	1.92	Γ_1^+
icsd_078869	CuF ₁₁ NaZr ₂	2	2.4	3.80	Γ_1^+
icsd_064660	CuF ₆ Pt	2	2.4	1.71	Γ_1^+
icsd_036514	CuF ₆ Sn	2	2.4	3.37	Γ_1^+
icsd_030117	CuF ₆ Zr	2	2.4	3.49	Γ_1^+
icsd_200533	CuFNbO ₃	2	2.4	2.35	Γ_1^+
icsd_085404	CuK ₆ O ₈ Si ₂	2	2.4	1.96	Γ_1^+
icsd_092854	CuLi ₂ O ₈ W ₂	2	2.4	2.03	Γ_1^+
icsd_002896	CuO ₆ S ₂ Tl ₂	2	2.4	1.13	Γ_1^+
icsd_028151	CuO ₆ V ₂	2	2.4	1.63	Γ_1^+
icsd_085405	CuO ₇ Rb ₄ Si ₂	2	2.4	2.09	Γ_1^+
icsd_411522	F ₁₂ MnSb ₂	2	2.4	3.69	Γ_1^+
icsd_171656	F ₆ O ₂ Rh	2	2.4	0.00	Γ_1^+
icsd_059585	FeNa ₄ O ₄	2	2.4	0.59	Γ_1^+
icsd_184601	FLiO ₄ PV	2	2.4	2.03	Γ_1^+
icsd_068184	H ₂ CuO ₅ S	2	2.4	2.07	Γ_1^+
icsd_039887	H ₂ CuO ₅ Se	2	2.4	2.33	Γ_1^+
icsd_069994	H ₂ O ₅ SeV	2	2.4	2.39	Γ_1^+
icsd_156225	H ₄ Ca ₂ MnO ₁₀ P ₂	2	2.4	4.22	Γ_1^+
icsd_098686	H ₄ CoK ₂ O ₁₀ Se ₂	2	2.4	3.74	Γ_1^+
icsd_098683	H ₄ CoNa ₂ O ₁₀ Se ₂	2	2.4	3.54	Γ_1^+
icsd_087958	H ₄ FeK ₂ O ₁₀ S ₂	2	2.4	3.99	Γ_1^+
icsd_096783	H ₄ K ₂ MnO ₁₀ Se ₂	2	2.4	3.25	Γ_1^+
icsd_098684	H ₄ Na ₂ NiO ₁₀ Se ₂	2	2.4	3.44	Γ_1^+
icsd_072461	H ₆ CuN ₄ O ₄	2	2.4	1.39	Γ_1^+
icsd_280299	H ₈ CdCl ₄ CuO ₄	2	2.4	1.59	Γ_1^+
icsd_080430	KMnO ₈ Se ₂	2	2.4	1.43	Γ_1^+
icsd_077829	LaSe	2	2.4	0.00	Γ_1^+
icsd_092853	Li ₂ NiO ₈ W ₂	2	2.4	2.90	Γ_1^+
icsd_189335	MoO ₆ Sr ₂ Ti	2	2.4	0.00	Γ_1^+
icsd_260257	NiO ₁₀ Te ₂ V ₂	2	2.4	2.00	Γ_1^+
icsd_001501	O ₂ V	2	2.4	0.00	Γ_1^+
icsd_415445	O ₅ PSnV	2	2.4	1.10	Γ_1^+
icsd_099699	BaMn ₂ O ₆ Y	3	3.3	0.00	Γ_2
icsd_670113	CuFO ₂	4	4.7	0.74	Γ_1
icsd_093022	O ₇ P ₂ V	4	4.9	1.69	Γ_2
icsd_068143	AgP ₂ Se ₆ V	5	5.13	0.39	Γ_1

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.075180	As ₂ FeLiO ₇	5	5.13	2.54	Γ_1
icsd.084683	B ₂ BaCuO ₅	5	5.15	2.22	Γ_2
icsd.046003	CoO ₆ V ₂	5	5.15	2.28	Γ_2
icsd.260893	CrCsP ₂ S ₇	5	5.15	1.68	Γ_2
icsd.091754	CrKP ₂ S ₇	5	5.15	1.70	Γ_2
icsd.059910	CsP ₂ S ₇ V	5	5.15	1.54	Γ_2
icsd.021067	CuO ₆ V ₂	5	5.13	1.25	Γ_1
icsd.039871	HCsMnO ₁₀ P ₃	5	5.15	1.13	Γ_2
icsd.091756	KP ₂ S ₇ V	5	5.15	1.50	Γ_2
icsd.073782	P ₂ RbS ₇ V	5	5.15	1.52	Γ_2
icsd.068713	S ₂ V	5	5.13	0.00	Γ_1
icsd.168320	BiFeO ₃	8	8.34	1.49	Γ_2
icsd.095439	Ca ₂ CoO 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 ₂ Se ₄	8	8.34	0.00	Γ_2
icsd.169981	HNiO ₂	8	8.32	0.00	Γ_1
icsd.645393	Nb ₂ Se ₄ Ti	8	8.34	0.00	Γ_2
icsd.645398	Nb ₂ Se ₄ V	8	8.32	0.00	Γ_1
icsd.023174	CaCrF ₅	9	9.37	2.22	Γ_1
icsd.169098	MoO ₅ P	9	9.37	0.12	Γ_1
icsd.150279	AuCrTe ₄	10	10.42	0.00	Γ_1^+
icsd.028909	CrO ₃ Y	10	10.46	1.20	Γ_2^+
icsd.001503	O ₂ V	10	10.46	0.00	Γ_2^+
icsd.089471	O ₂ V	10	10.46	1.07	Γ_2^+
icsd.246090	Ca ₂ MnO ₆ Sb	11	11.54	0.00	Γ_2^+
icsd.246091	Ca ₂ MnO ₆ Ta	11	11.54	0.00	Γ_2^+
icsd.084827	CoHf ₂ P	11	11.54	0.00	Γ_2^+
icsd.018176	CoO ₄ S	11	11.54	0.00	Γ_2^+
icsd.002232	CuI ₂ O ₆	11	11.50	2.15	Γ_1^+
icsd.170771	MnNaO ₄ Rb ₂	11	11.54	1.91	Γ_2^+
icsd.172559	Ag ₂ NiO 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 ₄ Mn	12	12.62	0.00	Γ_2^+
icsd.021055	Ba ₂ CuF ₆	12	12.62	2.18	Γ_2^+
icsd.174141	Ba ₂ IrLaO ₆	12	12.58	0.38	Γ_1^+
icsd.023903	Br ₂ Cr	12	12.62	1.08	Γ_2^+
icsd.022079	Br ₂ Cu	12	12.62	0.26	Γ_2^+
icsd.250692	C ₂ CoN ₂ S ₂	12	12.58	1.83	Γ_1^+
icsd.031320	C ₂ N ₂ NiS ₂	12	12.62	1.61	Γ_2^+
icsd.617514	C ₃ Cr ₂ Lu ₂	12	12.62	0.00	Γ_2^+
icsd.617562	C ₃ Cr ₂ Y ₂	12	12.62	0.00	Γ_2^+
icsd.160557	Ca ₂ CoO ₃	12	12.58	0.00	Γ_1^+
icsd.670347	CaMnO ₃	12	12.62	0.00	Γ_2^+
icsd.026667	Cl ₂ Cu	12	12.62	0.97	Γ_2^+
icsd.022080	Cl ₃ Cr	12	12.62	2.17	Γ_2^+
icsd.403035	Cl ₄ CrLi ₂	12	12.62	1.40	Γ_2^+
icsd.623661	Co ₂ Ge ₄ Y ₃	12	12.58	0.00	Γ_1^+
icsd.099989	Co ₃ Se ₄	12	12.62	0.00	Γ_2^+
icsd.623472	CoGe ₂ Lu 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 ₃ Sr ₂	12	12.62	0.00	Γ_2^+
icsd.169194	CoO ₆ Pb ₂ Te	12	12.62	1.22	Γ_2^+
icsd.077912	CoO ₆ Pb ₂ W	12	12.58	1.87	Γ_1^+
icsd.188911	CoO ₆ V ₂	12	12.62	2.25	Γ_2^+
icsd.624816	CoRh ₂ Se ₄	12	12.62	0.00	Γ_2^+
icsd.041746	CoSc ₂ Si ₂	12	12.58	0.00	Γ_1^+
icsd.624999	CoSe ₄ Si ₂	12	12.62	0.00	Γ_2^+
icsd.002371	CoSi ₂ Zr 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 ₂ MnS ₄	12	12.58	0.00	Γ_1^+
icsd.626299	Cr ₂ MnSe ₄	12	12.62	0.00	Γ_2^+

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.626640	Cr ₂ S ₄ Ti	12	12.62	0.00	Γ_2^+
icsd.626896	Cr ₂ Te ₄ Ti	12	12.62	0.00	Γ_2^+
icsd.626901	Cr ₂ Te ₄ V	12	12.62	0.00	Γ_2^+
icsd.016722	Cr ₃ S ₄	12	12.62	0.00	Γ_2^+
icsd.026976	Cr ₃ Se ₄	12	12.58	0.00	Γ_1^+
icsd.626873	Cr ₃ Te ₄	12	12.58	0.00	Γ_1^+
icsd.169764	CrF ₃ K	12	12.62	1.11	Γ_2^+
icsd.151873	CrFe ₂ Se 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 ₂ Se ₄	12	12.62	0.00	Γ_2^+
icsd.626579	CrRh ₂ Te 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 ₄ IrO ₄	12	12.62	0.58	Γ_2^+
icsd.066509	Cu ₂ Li ₃ O ₄	12	12.62	0.00	Γ_2^+
icsd.670115	CuHgO ₂	12	12.62	0.47	Γ_2^+
icsd.174134	CuLi ₂ O 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 ₂ Se ₄ V	12	12.58	0.00	Γ_1^+
icsd.427606	FeLa ₂ O ₂ Se ₂	12	12.62	2.31	Γ_2^+
icsd.022085	H ₄ Br ₂ CoO ₂	12	12.58	2.48	Γ_1^+
icsd.022084	H ₄ Br ₂ MnO ₂	12	12.58	3.00	Γ_1^+
icsd.022082	H ₄ Cl ₂ CoO ₂	12	12.58	3.16	Γ_1^+
icsd.015597	H ₄ Cl ₂ FeO ₂	12	12.62	3.20	Γ_2^+
icsd.015596	H ₄ Cl ₂ MnO ₂	12	12.58	4.07	Γ_1^+
icsd.009485	H ₄ CuF ₂ O ₂	12	12.62	3.16	Γ_2^+
icsd.260368	H ₄ O ₁₀ V ₄	12	12.58	1.07	Γ_2^+
icsd.047223	IrK ₄ O 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 ₆ V ₂	12	12.62	1.63	Γ_2^+
icsd.201787	Mo ₂ S ₄ V	12	12.62	0.00	Γ_2^+
icsd.026609	NaNiO ₂	12	12.58	0.16	Γ_1^+
icsd.182323	NaO ₂ V	12	12.58	1.83	Γ_1^+
icsd.076548	NaSe ₂ V	12	12.62	0.29	Γ_2^+
icsd.645395	Nb ₂ Se ₄ Ti	12	12.62	0.00	Γ_2^+
icsd.645402	Nb ₂ Se ₄ V	12	12.58	0.00	Γ_1^+
icsd.076670	NiO	12	12.62	1.75	Γ_2^+
icsd.016225	NiO ₆ Sr ₂ Te	12	12.62	2.10	Γ_2^+
icsd.015214	NiRh ₂ Se ₄	12	12.62	0.00	Γ_2^+
icsd.646533	NiSe ₄ Si ₂	12	12.62	0.00	Γ_2^+
icsd.084195	Se ₄ V ₃	12	12.62	0.00	Γ_2^+
icsd.038369	Te ₂ V _{1.04}	12	12.58	0.00	Γ_1^+
icsd.653087	Te ₄ TiV ₂	12	12.58	0.00	Γ_1^+
icsd.052510	Te ₄ V ₃	12	12.62	0.00	Γ_2^+
icsd.246938	BaCoS ₂	13	13.69	0.00	Γ_2^+
icsd.169005	CuO ₄ W	13	13.65	1.16	Γ_1^+
icsd.170685	MnO ₄ Re	13	13.69	0.00	Γ_1^+
icsd.093880	AgCuO ₂	14	14.75	0.00	Γ_1^+
icsd.421461	AgF ₄ K ₂	14	14.79	0.98	Γ_2^+
icsd.153857	Bi ₂ MnNiO ₆	14	14.75	0.27	Γ_1^+
icsd.290790	Ca ₂ CrO ₆ Sb	14	14.79	1.68	Γ_2^+
icsd.150696	Ca ₂ FeO ₆ Re	14	14.75	0.00	Γ_1^+
icsd.247998	Ca ₂ MnO ₆ Re	14	14.79	0.00	Γ_1^+
icsd.084791	Ca ₃ O ₆ Re	14	14.79	0.00	Γ_2^+
icsd.092336	CaFeO ₃	14	14.79	0.00	Γ_2^+
icsd.182568	CaO ₆ ReSr ₂	14	14.75	0.00	Γ_1^+
icsd.066201	Cl ₄ CrNa ₂	14	14.79	1.61	Γ_2^+
icsd.151837	CoLa ₂ MnO ₆	14	14.79	0.00	Γ_2^+
icsd.188982	CoMnO ₆ Y ₂	14	14.75	1.15	Γ_1^+
icsd.173491	CoO ₆ ReSr ₂	14	14.79	0.00	Γ_2^+
icsd.097662	CoO ₆ Sr ₂ W	14	14.79	2.10	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_042614	CoSb ₂	14	14.75	0.00	Γ_1^+
icsd_067250	CrF ₄ Na ₂	14	14.79	2.06	Γ_2^+
icsd_010350	CrF ₆ Li ₂	14	14.75	1.11	Γ_1^+
icsd_027070	CrF ₆ Na ₃	14	14.79	3.54	Γ_2^+
icsd_191374	CrMnO ₆ Y ₂	14	14.79	0.21	Γ_2^+
icsd_290789	CrO ₆ SbSr ₂	14	14.75	1.10	Γ_1^+
icsd_096085	CuGeO ₃	14	14.75	1.74	Γ_1^+
icsd_062655	F ₄ LiMn	14	14.79	2.09	Γ_2^+
icsd_071455	F ₄ MnNa	14	14.79	2.31	Γ_2^+
icsd_290251	F ₆ Li ₂ V	14	14.75	2.69	Γ_1^+
icsd_066315	F ₆ MnNa ₃	14	14.79	1.66	Γ_2^+
icsd_026073	F ₆ Na ₃ Ni	14	14.79	2.20	Γ_2^+
icsd_027347	F ₆ Na ₃ V	14	14.79	2.50	Γ_2^+
icsd_095517	FeO ₆ Sr ₂ W	14	14.79	1.35	Γ_2^+
icsd_237528	In ₂ MnNiO ₆	14	14.79	1.74	Γ_2^+
icsd_203219	La ₂ LiMoO ₆	14	14.79	0.51	Γ_2^+
icsd_186428	La ₂ MnNiO ₆	14	14.79	0.15	Γ_2^+
icsd_163761	La ₂ MnO ₆ V	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 ₃ Y	14	14.79	1.78	Γ_2^+
icsd_251832	MnNiO ₆ Sc ₂	14	14.79	1.99	Γ_2^+
icsd_192872	MnNiO ₆ Y ₂	14	14.79	0.96	Γ_2^+
icsd_251022	MnO ₃ Sc	14	14.75	0.91	Γ_1^+
icsd_069801	MnO ₆ Se ₂	14	14.75	1.56	Γ_1^+
icsd_095948	NiO ₃ Tl	14	14.79	0.00	Γ_2^+
icsd_088043	NiO ₃ Y	14	14.79	0.23	Γ_2^+
icsd_150258	LaMnO ₃	15	15.85	0.00	Γ_1^+
icsd_063230	BaS ₃ V	20	20.34	0.00	Γ_3^+
icsd_077832	S ₂ V	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 ₄ Si	31	31.125	0.00	Γ_4^+
icsd_002257	HCrO ₂	31	31.125	2.02	Γ_4^+
icsd_088640	LiO ₅ V ₂	31	31.125	1.52	Γ_4^+
icsd_047101	MnNa ₅ O ₄	31	31.127	1.45	Γ_2^+
icsd_236365	MnO ₃ Y	31	31.125	0.49	Γ_4^+
icsd_001898	NaO ₅ V 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 ₃ V	36	36.176	0.00	Γ_2^+
icsd_002596	CrI ₂	36	36.174	0.00	Γ_4^+
icsd_068459	H ₂ CuO ₂	36	36.176	1.81	Γ_2^+
icsd_000284	MgO ₃ V	36	36.174	2.78	Γ_4^+
icsd_617417	C ₂ CoLu	38	38.190	0.00	Γ_3^+
icsd_057007	C ₂ CoY	38	38.189	0.00	Γ_4^+
icsd_617756	C ₂ FeLu	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 ₂ Cu ₃ LaO ₈	47	47.252	0.00	Γ_2^+
icsd_164176	BaFe ₂ O ₅ Y	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 ₂ Ge ₂ Ni ₃	51	51.295	0.00	Γ_3^+
icsd_623100	Co ₂ GaLa	51	51.296	0.00	Γ_4^+
icsd_658677	Co ₂ InY	51	51.295	0.00	Γ_3^+
icsd_190616	Co ₂ NbSn	51	51.295	0.00	Γ_3^+
icsd_071520	FeNbTe ₂	53	53.328	0.00	Γ_4^+
icsd_015087	H ₄ Cl ₂ CuO ₂	53	53.328	2.03	Γ_4^+
icsd_083907	CrLaSb ₃	57	57.383	0.00	Γ_3^+
icsd_610034	As ₂ Co	58	58.398	0.00	Γ_3^+
icsd_236413	C ₂ H ₂ CoN ₄	58	58.397	2.24	Γ_2^+
icsd_172908	C ₂ H ₂ N ₄ Ni	58	58.398	2.53	Γ_4^+

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_015467	Cl ₂ Cr	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 ₂ Ru	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 ₂ MgO ₃	59	59.409	0.59	Γ_3^+
icsd_095957	Cu ₂ O ₃ Sr	59	59.409	0.00	Γ_2^+
icsd_088639	LiO ₅ V ₂	59	59.409	0.35	Γ_2^+
icsd_059345	NaO ₅ V 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 ₂ Fe	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_4^+
icsd_092330	CaFeO ₃	62	62.446	0.00	Γ_2^+
icsd_670820	CaI ₂ Fe	62	62.447	0.00	Γ_3^+
icsd_237732	CaO ₃ Os	62	62.446	0.00	Γ_2^+
icsd_164775	CaO ₃ Rh	62	62.447	0.03	Γ_3^+
icsd_088387	CdO ₃ V	62	62.448	1.70	Γ_4^+
icsd_187138	CFe ₂	62	62.448	0.00	Γ_4^+
icsd_670832	CFe ₂ Si	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 ₃ Sb	62	62.447	0.88	Γ_3^+
icsd_084866	CrSbSe ₃	62	62.446	0.50	Γ_2^+
icsd_000498	CuO ₃ Se	62	62.446	1.60	Γ_2^+
icsd_029338	CuO ₃ Te	62	62.448	1.48	Γ_4^+
icsd_633291	Fe ₃ S	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 ₃ Y	62	62.447	0.17	Γ_3^+
icsd_041149	MnRhSi	62	62.446	0.00	Γ_2^+
icsd_093507	NiO ₃ Tl	62	62.446	0.00	Γ_2^+
icsd_191794	NiO ₃ Y	62	62.446	0.00	Γ_2^+
icsd_022303	O ₂ V	62	62.448	0.38	Γ_4^+
icsd_237731	O ₃ OsSr	62	62.447	0.00	Γ_3^+
icsd_008150	O ₃ TiY	62	62.446	2.09	Γ_2^+
icsd_043686	PRu ₂	62	62.447	0.00	Γ_3^+

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)	Irrrep
icsd_105931	Rh ₂ Sn	62	62.447	0.00	Γ_3^+
icsd_670862	Rh ₃ Si	62	62.446	0.00	Γ_2^+
icsd_108723	RhSiTi	62	62.448	0.00	Γ_4^+
icsd_057645	Al ₂ CoY	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 ₃ Rh	63	63.464	0.00	Γ_4^+
icsd_656056	Cs ₂ NiP ₂	63	63.464	0.29	Γ_4^+
icsd_016217	CuO ₂ Sr	63	63.463	0.30	Γ_3^+
icsd_632057	FeGe ₂ Lu	63	63.462	0.00	Γ_2^+
icsd_632162	FeGe ₂ Y	63	63.462	0.00	Γ_2^+
icsd_637012	GeMnNi	63	63.462	0.00	Γ_2^+
icsd_036123	NiO ₂ Sr	63	63.463	0.76	Γ_3^+
icsd_043843	Al ₂ B ₂ Ru ₃	65	65.486	0.00	Γ_3^+
icsd_020083	AlB ₂ Cr ₂	65	65.486	0.00	Γ_3^+
icsd_020322	AlB ₂ Fe ₂	65	65.485	0.00	Γ_2^+
icsd_025518	AlB ₂ Mn ₂	65	65.486	0.00	Γ_4^+
icsd_082199	Br ₄ FeLi ₂	65	65.486	3.09	Γ_3^+
icsd_033865	Br ₄ Li ₂ Mn	65	65.486	3.67	Γ_3^+
icsd_073227	Cl ₄ CoLi ₂	65	65.486	2.59	Γ_3^+
icsd_001165	Cl ₄ Os	65	65.486	0.76	Γ_4^+
icsd_072872	CoO ₄ Re	65	65.486	0.00	Γ_4^+
icsd_035338	CoO ₆ Pt ₃	65	65.485	0.40	Γ_2^+
icsd_174117	CuF ₄ K ₂	65	65.486	2.17	Γ_3^+
icsd_015927	MgO ₃ V	65	65.485	0.00	Γ_2^+
icsd_035337	MnO ₆ Pt ₃	65	65.486	0.39	Γ_3^+
icsd_078012	AlF ₅ Fe	71	71.536	4.32	Γ_3^+
icsd_613166	B ₂ CoMo ₂	71	71.536	0.00	Γ_2^+
icsd_016776	B ₂ CoW ₂	71	71.536	0.00	Γ_2^+
icsd_614261	B ₂ FeW ₂	71	71.536	0.00	Γ_2^+
icsd_033704	B ₄ Cr ₃	71	71.536	0.00	Γ_4^+
icsd_614775	B ₄ Mn ₂ Ta	71	71.536	0.00	Γ_2^+
icsd_614782	B ₄ Mn ₂ W	71	71.536	0.00	Γ_2^+
icsd_044446	B ₄ Mn ₃	71	71.536	0.00	Γ_2^+
icsd_068795	BaNiO ₅ Y ₂	71	71.536	2.09	Γ_3^+
icsd_024381	Br ₂ OV	71	71.536	0.57	Γ_4^+
icsd_040950	C ₄ CoSc ₃	71	71.536	0.00	Γ_4^+
icsd_072863	C ₄ FeSc ₃	71	71.536	0.00	Γ_2^+
icsd_016216	Ca ₂ CuO ₃	71	71.536	0.37	Γ_2^+
icsd_024380	Cl ₂ OV	71	71.536	0.76	Γ_4^+
icsd_025001	CuLi ₂ O ₂	71	71.536	1.36	Γ_3^+
icsd_015127	CuO ₃ Sr ₂	71	71.536	0.20	Γ_2^+
icsd_068700	FeLi ₄ N ₂	71	71.536	0.94	Γ_3^+
icsd_251018	FeO ₃ Sr ₂	71	71.536	1.01	Γ_2^+
icsd_188992	GaMnNi ₂	71	71.536	0.00	Γ_3^+
icsd_167658	H ₂ PdTi ₂	71	71.536	0.00	Γ_3^+
icsd_416513	CoPd ₂ Se ₂	72	72.544	0.00	Γ_4^+
icsd_416514	CoPd ₂ Te ₂	72	72.543	0.00	Γ_2^+
icsd_416515	FePd ₂ Se ₂	72	72.544	0.00	Γ_3^+
icsd_670341	CaMnO ₃	74	74.559	0.22	Γ_3^+
icsd_036535	Cu ₂ O ₂ Tl	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 ₂ FeS ₄ Sn	81	3.3	0.65	$\Gamma_3\Gamma_4$
icsd_052961	CoGa ₂ S ₄	82	82.39	1.80	Γ_1
icsd_152909	Ga ₂ MnS ₄	82	82.39	1.71	Γ_1
icsd_000415	Ga ₂ MnSe ₄	82	82.39	1.54	Γ_1
icsd_018307	O ₅ SV	85	85.59	2.18	Γ_1^+
icsd_611737	Au ₄ Cr	87	12.62	0.00	$\Gamma_3^+\Gamma_4^+$
icsd_107998	Au ₄ Mn	87	87.75	0.00	Γ_1^+
icsd_612460	Au ₄ V	87	87.75	0.00	Γ_1^+
icsd_171987	Ba ₂ CaO ₆ Re	87	12.62	0.00	$\Gamma_3^+\Gamma_4^+$
icsd_191960	Ba ₂ CuO ₆ Os	87	12.62	0.10	$\Gamma_3^+\Gamma_4^+$
icsd_088703	Ba ₂ CuO ₆ Te	87	87.75	0.76	Γ_1^+
icsd_072813	Ba ₂ CuO ₆ W	87	87.75	1.39	Γ_1^+

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_095518	Ba ₂ FeO ₆ W	87	12.62	1.30	$\Gamma_3^+ \Gamma_4^+$
icsd_192904	Ca ₂ MnO ₆ Ti	87	12.62	1.28	$\Gamma_3^+ \Gamma_4^+$
icsd_262352	Co _{0.5} O ₃ Re _{0.5} Sr	87	12.62	0.00	$\Gamma_3^+ \Gamma_4^+$
icsd_153544	CoMoO ₆ Sr ₂	87	12.62	1.30	$\Gamma_3^+ \Gamma_4^+$
icsd_192327	CoNbO ₆ Sr ₂	87	12.62	0.60	$\Gamma_3^+ \Gamma_4^+$
icsd_173488	CoO ₆ ReSr ₂	87	12.62	0.00	$\Gamma_3^+ \Gamma_4^+$
icsd_190593	CoO ₆ Sr ₂ W	87	12.62	2.12	$\Gamma_3^+ \Gamma_4^+$
icsd_186038	CuMoO ₆ Sr ₂	87	87.75	1.46	Γ_1^+
icsd_033573	CuO ₆ Sr ₂ Te	87	87.75	1.54	Γ_1^+
icsd_033571	CuO ₆ Sr ₂ W	87	87.75	1.74	Γ_1^+
icsd_150702	FeO ₆ ReSr ₂	87	12.62	0.00	$\Gamma_3^+ \Gamma_4^+$
icsd_078677	FeO ₆ Sr ₂ W	87	12.62	0.00	$\Gamma_3^+ \Gamma_4^+$
icsd_067826	IrNa ₄ O ₄	87	87.75	0.74	Γ_1^+
icsd_250818	IrNiO ₆ Sr ₂	87	12.62	0.25	$\Gamma_3^+ \Gamma_4^+$
icsd_194696	MgO ₆ OsSr ₂	87	12.62	0.00	$\Gamma_3^+ \Gamma_4^+$
icsd_182569	MgO ₆ ReSr ₂	87	87.75	0.00	Γ_1^+
icsd_187669	MnMoO ₆ Sr ₂	87	12.62	0.81	$\Gamma_3^+ \Gamma_4^+$
icsd_098191	MoNiO ₆ Sr ₂	87	12.62	2.12	$\Gamma_3^+ \Gamma_4^+$
icsd_152440	NiO ₆ OsSr ₂	87	12.62	0.00	$\Gamma_3^+ \Gamma_4^+$
icsd_173487	NiO ₆ ReSr ₂	87	87.75	0.00	Γ_1^+
icsd_009294	NiO ₆ Sr ₂ W	87	12.62	2.96	$\Gamma_3^+ \Gamma_4^+$
icsd_173489	O ₆ ReSr ₂ Zn	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 ₄ Cl ₂ CuO ₄ Pb ₂	99	99.167	2.06	Γ_4^+
icsd_152276	O ₃ PbV	99	99.167	1.32	Γ_4^+
icsd_042373	CoGe ₃ La	107	107.231	0.00	Γ_4^+
icsd_059908	FeGe ₃ La	107	107.231	0.00	Γ_4^+
icsd_039351	MnO ₆ SbSr ₂	107	107.231	0.09	Γ_4^+
icsd_631817	FeGa ₂ Se 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 ₂ Tl	119	119.319	0.00	Γ_3^+
icsd_633509	FeSe ₂ Tl	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 ₂ FeS ₄ Sn	121	23.51	0.03	Γ_5^+
icsd_608538	Al ₂ MnTe ₄	121	42.221	0.88	Γ_5^+
icsd_016809	BFe ₂	121	23.51	0.00	Γ_5^+
icsd_099293	CoCu ₂ GeS ₄	121	121.331	0.70	Γ_4^+
icsd_099292	CoCu ₂ S ₄ Si	121	23.51	1.11	Γ_5^+
icsd_099294	CoCu ₂ S ₄ Sn	121	121.331	0.71	Γ_4^+
icsd_099296	CoCu ₂ Se ₄ Sn	121	121.331	0.19	Γ_4^+
icsd_108934	CrK ₃ O ₄	121	42.221	0.89	Γ_5^+
icsd_047165	Cu ₂ FeGeS ₄	121	23.51	1.02	Γ_5^+
icsd_627313	Cu ₂ FeGeSe ₄	121	42.221	0.44	Γ_5^+
icsd_026721	Cu ₂ FeS ₄ Sn	121	42.221	0.78	Γ_5^+
icsd_627368	Cu ₂ FeSe ₄ Si	121	23.51	0.98	Γ_5^+
icsd_085126	Cu ₂ FeSe ₄ Sn	121	23.51	0.23	Γ_5^+
icsd_042489	Cu ₂ MnS ₄ Sn	121	121.331	0.72	Γ_4^+
icsd_155904	Cu ₂ MnSe ₄ Sn	121	121.331	0.12	Γ_4^+
icsd_659100	Ga ₂ MnSe ₄	121	42.221	0.42	Γ_5^+
icsd_172506	GeMnTe ₄ Tl ₂	121	121.331	0.13	Γ_4^+
icsd_639984	In ₂ MnTe ₄	121	42.221	0.47	Γ_5^+
icsd_108935	K ₃ MnO ₄	121	42.221	1.86	Γ_5^+
icsd_172507	MnSnTe ₄ Tl ₂	121	121.331	0.26	Γ_4^+
icsd_107862	AlNi ₃	123	65.486	0.00	Γ_5^+
icsd_169074	As ₂ BaOTi 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 ₂ Ca ₂ Cu ₃ HgO ₈	123	123.345	0.00	Γ_3^+
icsd_074163	Ba ₂ Cu ₂ O ₇ TlY	123	65.486	0.00	Γ_5^+
icsd_075720	Ba ₂ CuHgO ₄	123	123.345	0.00	Γ_3^+
icsd_430063	BaBi ₂ OTi ₂	123	47.252	0.00	Γ_5^+

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_028918	BaFeO ₃	123	123.345	0.00	Γ_3^+
icsd_150703	BaLaMn ₂ O ₆	123	47.252	0.00	Γ_5^+
icsd_237789	BaOSb ₂ Ti ₂	123	47.252	0.00	Γ_5^+
icsd_088033	BrCuLaNb ₂ O ₇	123	47.252	0.03	Γ_4^+
icsd_051262	Ca ₂ ClCuNb ₃ O 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 ₂ O ₇	123	47.252	0.76	Γ_5^+
icsd_051261	ClCuLaO ₇ Ta ₂	123	47.252	0.29	Γ_5^+
icsd_157788	Co ₂ GaNi	123	65.486	0.00	Γ_5^+
icsd_623081	CoGa ₄ Hf	123	65.486	0.00	Γ_5^+
icsd_623236	CoGa ₅ Y	123	123.345	0.00	Γ_3^+
icsd_623111	CoGa ₈ Lu ₂	123	65.486	0.00	Γ_5^+
icsd_623237	CoGa ₈ Y ₂	123	123.345	0.00	Γ_3^+
icsd_150261	CoIn ₅ La	123	47.252	0.00	Γ_5^+
icsd_623947	CoIn ₅ Y	123	47.252	0.00	Γ_5^+
icsd_623948	CoIn ₈ Y ₂	123	47.252	0.00	Γ_5^+
icsd_412978	CoNa ₅ O ₂ S	123	47.252	1.16	Γ_5^+
icsd_027690	CrF ₃ K	123	47.252	0.00	Γ_5^+
icsd_069675	Cs ₂ F ₅ Mn	123	123.345	1.56	Γ_3^+
icsd_027689	CuF ₃ K	123	65.486	1.55	Γ_5^+
icsd_109293	CuF ₃ Rb	123	65.486	1.60	Γ_5^+
icsd_043457	CuF ₃ Tl	123	65.486	0.76	Γ_5^+
icsd_021072	F ₄ FeRb	123	47.252	2.13	Γ_5^+
icsd_082218	F ₅ MnRb ₂	123	123.345	1.47	Γ_3^+
icsd_186722	Fe ₂ GaMn	123	123.345	0.00	Γ_3^+
icsd_600147	FeGa ₈ Lu ₂	123	47.252	0.00	Γ_5^+
icsd_173434	FeO ₂ Sr	123	65.486	0.00	Γ_5^+
icsd_184861	FeO ₃ Sr	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 ₂ Sb	123	47.252	0.00	Γ_5^+
icsd_412972	Na ₅ NiO ₂ S	123	123.345	1.47	Γ_3^+
icsd_028837	OPd	123	47.252	0.00	Γ_5^+
icsd_623784	CoHf ₄ P	124	124.357	0.00	Γ_3^+
icsd_632255	FeHf ₄ P	124	66.496	0.00	Γ_5^+
icsd_632795	FeNb ₄ P	124	66.496	0.00	Γ_5^+
icsd_053511	FeNb ₄ Si	124	66.496	0.00	Γ_5^+
icsd_613529	B ₂ CrNb ₂	127	65.486	0.00	Γ_5^+
icsd_613557	B ₂ CrTa ₂	127	65.486	0.00	Γ_5^+
icsd_044449	B ₂ MnW ₂	127	55.358	0.00	Γ_5^+
icsd_615683	B ₄ W	127	127.393	0.00	Γ_3^+
icsd_249632	Ga ₅ Mn ₂	127	65.486	0.00	Γ_5^+
icsd_104026	Ga ₅ V ₂	127	55.358	0.00	Γ_5^+
icsd_245749	Cl ₆ K ₂ Nb	128	58.398	0.06	Γ_5^+
icsd_042750	AlGeMn	129	129.417	0.00	Γ_3^+
icsd_262356	As ₂ Co ₂ O ₆ Sc ₂ Sr ₄	129	67.506	0.00	Γ_5^+
icsd_610777	As ₂ LaRh 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 ₂ CoSc	129	129.417	0.00	Γ_3^+
icsd_617820	C ₂ FeSc	129	59.410	0.00	Γ_5^+
icsd_085283	CBNiY	129	59.410	0.00	Γ_5^+
icsd_090122	ClCoO ₃ Sr ₂	129	67.506	0.00	Γ_5^+
icsd_050988	ClKMoO ₅ P	129	129.417	1.36	Γ_3^+
icsd_094745	ClMnO ₃ Sr ₂	129	129.417	0.00	Γ_3^+
icsd_050989	ClMoO ₅ PRb	129	129.417	1.30	Γ_3^+
icsd_237581	ClNiO ₃ Sr 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 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_191258	CrN ₃ Nb	129	129.417	0.00	Γ_3^+
icsd_091199	CuMnO ₃ SSr 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 ₂ O ₅ V	129	129.417	2.33	Γ_3^+
icsd_085904	GeTiY	129	59.410	0.00	Γ_5^+
icsd_059359	Li ₂ O ₅ SiV	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 ₂ Sr ₂	136	136.501	0.32	Γ_3^+
icsd_108964	CoO ₆ Sb ₂	136	65.486	0.93	Γ_5^+
icsd_173874	Cr ₂ O ₆ Re	136	136.501	0.00	Γ_3^+
icsd_009423	CrO ₂	136	136.501	0.00	Γ_3^+
icsd_130032	Cu ₂ Hf ₂ In	136	136.501	0.00	Γ_3^+
icsd_130034	Cu ₂ InZr ₂	136	136.501	0.00	Γ_3^+
icsd_290252	F ₆ Li ₂ V	136	136.501	2.21	Γ_3^+
icsd_035382	F ₆ LiV ₂	136	136.501	0.00	Γ_3^+
icsd_068525	Fe ₄ P ₂ Sc	136	58.398	0.00	Γ_5^+
icsd_633122	Fe ₄ P ₂ Zr	136	58.398	0.00	Γ_5^+
icsd_087172	Fe ₄ Si ₂ Zr	136	58.398	0.00	Γ_5^+
icsd_040344	FeO ₆ Sb ₂	136	58.398	0.06	Γ_5^+
icsd_189495	Ni ₄ P ₂ Y	136	38.190	0.00	Γ_3^+
icsd_080802	NiO ₆ Sb ₂	136	136.501	1.28	Γ_3^+
icsd_061198	NiO ₆ Ta ₂	136	136.501	2.91	Γ_3^+
icsd_076024	O ₂ Ta	136	136.501	0.00	Γ_3^+
icsd_001504	O ₂ V	136	136.501	0.74	Γ_3^+
icsd_238076	Ag ₂ Ba ₂ CoO ₂ Se ₂	139	71.536	0.50	Γ_5^+
icsd_016254	AgCs ₂ F ₄	139	69.524	0.00	Γ_5^+
icsd_609234	Al ₂ Ru	139	139.537	0.00	Γ_3^+
icsd_085659	As ₂ Ba ₂ MnO ₂ Zn ₂	139	69.524	0.00	Γ_5^+
icsd_610072	As ₂ Co ₂ K	139	139.537	0.00	Γ_3^+
icsd_610297	As ₂ CsRu ₂	139	139.537	0.00	Γ_3^+
icsd_167013	As ₂ F ₂ OSr ₂ Ti ₂	139	71.536	0.00	Γ_5^+
icsd_604549	B ₂ Fe ₂ Lu	139	139.537	0.00	Γ_3^+
icsd_614264	B ₂ Fe ₂ Y	139	139.537	0.00	Γ_3^+
icsd_054042	B ₂ La ₃ N ₃ Ni ₂	139	139.537	0.00	Γ_3^+
icsd_261352	Ba ₂ CoCu ₂ O ₂ S ₂	139	69.524	0.80	Γ_5^+
icsd_021057	Ba ₂ CoF ₆	139	69.524	3.39	Γ_5^+
icsd_033569	Ba ₂ CuO ₆ W	139	139.537	1.60	Γ_3^+
icsd_021056	Ba ₂ F ₆ Ni	139	139.537	3.94	Γ_3^+
icsd_155174	Ba ₂ FeO ₆ Re	139	139.537	0.00	Γ_3^+
icsd_420975	BaCo ₂ Ge ₂	139	139.537	0.00	Γ_3^+
icsd_001028	Br ₂ Ca ₂ CuO ₂	139	139.537	0.00	Γ_3^+
icsd_059698	Br ₂ CoO ₂ Sr ₂	139	69.524	1.11	Γ_5^+
icsd_008174	Br ₄ MnRb ₂	139	69.524	2.58	Γ_5^+
icsd_001027	Ca ₂ Cl ₂ CuO ₂	139	139.537	0.00	Γ_3^+
icsd_425467	CaFe ₂ Si ₂	139	71.536	0.00	Γ_5^+
icsd_059697	Cl ₂ CoO ₂ Sr ₂	139	69.524	1.04	Γ_5^+
icsd_004087	Cl ₂ CuO ₂ Sr ₂	139	139.537	0.00	Γ_3^+
icsd_041571	Cl ₄ CrCs ₂	139	71.536	0.00	Γ_5^+
icsd_009857	Cl ₄ CrRb ₂	139	139.537	0.00	Γ_3^+
icsd_001139	Cl ₄ MnRb ₂	139	71.536	3.35	Γ_5^+
icsd_245748	Cl ₆ NbRb ₂	139	69.524	0.00	Γ_5^+
icsd_081750	Co ₂ Ge ₂ La	139	139.537	0.00	Γ_3^+
icsd_623956	Co ₂ KS ₂	139	71.536	0.00	Γ_5^+
icsd_067370	Co ₂ KSe ₂	139	71.536	0.00	Γ_5^+
icsd_624795	Co ₂ RbS ₂	139	69.524	0.00	Γ_5^+
icsd_624798	Co ₂ RbSe ₂	139	69.524	0.00	Γ_5^+
icsd_067362	Co ₂ Se ₂ Tl	139	69.524	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_074889	CoCsK ₂ O ₂	139	69.524	1.93	Γ_5^+
icsd_033522	CoF ₄ K ₂	139	69.524	3.78	Γ_5^+
icsd_069683	CoF ₄ Rb ₂	139	69.524	3.84	Γ_5^+
icsd_670534	CoFeLa ₂ O ₆	139	139.537	1.81	Γ_3^+
icsd_191364	CoHfO ₆ Sr ₂	139	139.537	0.00	Γ_3^+
icsd_191362	CoLaO ₆ Sr ₂	139	71.536	0.62	Γ_5^+
icsd_053059	CoO	139	71.536	1.85	Γ_5^+
icsd_246483	CoO ₄ Sr ₂	139	71.536	0.00	Γ_5^+
icsd_405782	CoO ₆ Pb ₂ Te	139	71.536	2.06	Γ_5^+
icsd_191361	CoO ₆ Sr ₂ Y	139	71.536	0.32	Γ_5^+
icsd_191363	CoO ₆ Sr ₂ Zr	139	71.536	0.23	Γ_5^+
icsd_075384	CrF ₆ Nb	139	69.524	0.00	Γ_5^+
icsd_191358	CrHfO ₆ Sr ₂	139	71.536	0.00	Γ_5^+
icsd_191357	CrO ₆ Sr ₂ Zr	139	71.536	0.00	Γ_5^+
icsd_065259	Cs ₂ CuF ₆	139	69.524	0.31	Γ_5^+
icsd_039535	Cs ₂ CuO ₂	139	139.537	0.00	Γ_3^+
icsd_091036	Cs ₂ F ₆ KMn	139	139.537	1.75	Γ_3^+
icsd_423923	Cs ₂ NiO ₂	139	69.524	2.31	Γ_5^+
icsd_084734	Cu ₂ MnO ₂ S ₂ Sr ₂	139	69.524	0.00	Γ_5^+
icsd_088424	Cu ₂ NiO ₂ S ₂ Sr ₂	139	69.524	0.11	Γ_5^+
icsd_088423	Cu ₃ O ₂ S ₂ Sr ₂	139	139.537	0.00	Γ_3^+
icsd_015372	CuF ₄ K ₂	139	69.524	2.09	Γ_5^+
icsd_055710	CuI ₂ O ₂ Sr ₂	139	71.536	0.00	Γ_5^+
icsd_039475	CuIn ₂ O ₄	139	139.537	0.00	Γ_5^+
icsd_041643	CuLa ₂ O ₄	139	139.537	0.00	Γ_3^+
icsd_167014	F ₂ OSb ₂ Sr ₂ Ti ₂	139	71.536	0.00	Γ_5^+
icsd_023183	F ₄ K ₂ Mn	139	69.524	2.77	Γ_5^+
icsd_015576	F ₄ K ₂ Ni	139	139.537	3.85	Γ_3^+
icsd_023949	F ₄ Nb	139	139.537	0.00	Γ_3^+
icsd_069682	F ₄ NiRb ₂	139	139.537	3.89	Γ_3^+
icsd_009708	F ₆ MnNaRb ₂	139	139.537	1.65	Γ_3^+
icsd_081747	Fe ₂ Ge ₂ La	139	139.537	0.00	Γ_3^+
icsd_081745	Fe ₂ Ge ₂ Y	139	69.524	0.00	Γ_5^+
icsd_186572	Fe ₂ KS ₂	139	69.524	0.00	Γ_5^+
icsd_186573	Fe ₂ KSe ₂	139	71.536	0.00	Γ_5^+
icsd_186574	Fe ₂ KTe ₂	139	71.536	0.00	Γ_5^+
icsd_632475	Fe ₂ LuSi ₂	139	71.536	0.00	Γ_5^+
icsd_633338	Fe ₂ S ₂ Tl	139	139.537	0.00	Γ_3^+
icsd_053544	Fe ₂ Se ₂ Tl	139	139.537	0.00	Γ_3^+
icsd_191366	FeHfO ₆ Sr ₂	139	69.524	0.00	Γ_5^+
icsd_670535	FeIrLa ₂ O ₆	139	139.537	0.46	Γ_3^+
icsd_069849	FeO ₄ Sr ₂	139	71.536	0.00	Γ_5^+
icsd_191365	FeO ₆ Sr ₂ Zr	139	139.537	0.59	Γ_3^+
icsd_670137	Ga ₃ Mo	139	139.537	0.00	Γ_3^+
icsd_634592	Ga ₄ LuTi ₂	139	139.537	0.00	Γ_3^+
icsd_635352	Ga ₄ ScTi ₂	139	139.537	0.00	Γ_3^+
icsd_103999	Ga ₄ Ti ₂ Y	139	139.537	0.00	Γ_3^+
icsd_635567	Ga ₄ Ti ₂ Zr	139	139.537	0.00	Γ_3^+
icsd_153292	GaMnNi ₂	139	139.537	0.00	Γ_3^+
icsd_107040	Ge ₂ LuMn ₂	139	71.536	0.00	Γ_5^+
icsd_053715	Ge ₂ Mn ₂ Y	139	71.536	0.00	Γ_5^+
icsd_090234	GeTiY	139	69.524	0.00	Γ_5^+
icsd_168287	Hf ₂ Tl	139	71.536	0.00	Γ_5^+
icsd_191630	HfLa ₂ NiO ₆	139	71.536	1.64	Γ_5^+
icsd_191360	HfO ₆ Sr ₂ V	139	71.536	0.94	Γ_5^+
icsd_072191	I ₂ La	139	139.537	0.00	Γ_3^+
icsd_021069	K ₂ NiO ₂	139	71.536	2.37	Γ_5^+
icsd_181385	La ₂ Mn ₂ O ₃ Se ₂	139	69.524	1.79	Γ_5^+
icsd_001179	La ₂ NiO ₄	139	69.524	0.88	Γ_5^+
icsd_191628	La ₂ NiO ₆ Ti	139	71.536	2.32	Γ_5^+
icsd_191629	La ₂ NiO ₆ Zr	139	71.536	1.55	Γ_5^+
icsd_169470	La ₂ O ₆ ReV	139	139.537	0.14	Γ_3^+
icsd_090197	LuRu ₂ Si ₂	139	69.524	0.00	Γ_5^+
icsd_098525	MgO ₆ ReSr ₂	139	139.537	0.00	Γ_3^+
icsd_082937	Mn ₂ Si ₂ Y	139	71.536	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)	Irrrep
icsd_106932	MnN	139	69.524	0.00	Γ_5^+
icsd_026560	MnO ₄ Sr ₂	139	71.536	0.00	Γ_5^+
icsd_152123	MoO ₄ Sr ₂	139	69.524	0.00	Γ_5^+
icsd_073209	Na ₂ NiO ₂ Rb	139	139.537	1.52	Γ_3^+
icsd_069648	Na ₂ OSb ₂ Ti ₂	139	69.524	0.00	Γ_5^+
icsd_066277	NiO ₂ Rb ₂	139	69.524	2.45	Γ_5^+
icsd_239358	O ₄ RhSr ₂	139	139.537	0.00	Γ_3^+
icsd_033802	O ₄ RuSr ₂	139	139.537	0.00	Γ_3^+
icsd_236760	O ₄ Sr ₂ Tc	139	71.536	0.00	Γ_5^+
icsd_069000	O ₄ Sr ₂ V	139	139.537	0.00	Γ_3^+
icsd_191359	O ₆ Sr ₂ VZr	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 ₃ RuSr	140	140.547	0.00	Γ_3^+
icsd_031149	Fe ₂ Li ₂ O ₄	141	70.530	0.59	Γ_5^+
icsd_162264	BiFeO ₃	146	1.1	0.21	$\Gamma_2\Gamma_3$
icsd_193740	H ₄ As ₃ MnNS ₆	146	1.1	1.97	$\Gamma_2\Gamma_3$
icsd_091527	KNiO ₉ P ₃	146	146.10	4.55	Γ_1
icsd_408193	Ag ₂ BaMnO ₈ V ₂	147	2.4	2.43	$\Gamma_2^+\Gamma_3^+$
icsd_194590	Ag ₂ FeKO ₈ V ₂	147	2.4	2.02	$\Gamma_2^+\Gamma_3^+$
icsd_194588	Ag ₂ FeO ₈ RbV ₂	147	2.4	1.99	$\Gamma_2^+\Gamma_3^+$
icsd_429825	BaLi ₂ MnO ₈ V ₂	147	2.4	2.96	$\Gamma_2^+\Gamma_3^+$
icsd_051015	CoO ₈ Re ₂	147	2.4	2.20	$\Gamma_2^+\Gamma_3^+$
icsd_164948	CrO ₆ TeY	147	15.85	1.07	$\Gamma_2^+\Gamma_3^+$
icsd_245667	CsFeO ₈ S ₂	147	2.4	1.53	$\Gamma_2^+\Gamma_3^+$
icsd_073736	CsO ₈ S ₂ V	147	2.4	2.20	$\Gamma_2^+\Gamma_3^+$
icsd_245666	FeMo ₂ O ₈ Rb	147	2.4	2.54	$\Gamma_2^+\Gamma_3^+$
icsd_051014	MnO ₈ Re ₂	147	2.4	3.59	$\Gamma_2^+\Gamma_3^+$
icsd_051016	NiO ₈ Re ₂	147	147.13	2.47	Γ_1^+
icsd_260062	As ₂ BaCo ₂ O ₈	148	148.17	3.00	Γ_1^+
icsd_671511	AsInNi ₃	148	2.4	0.00	$\Gamma_2^+\Gamma_3^+$
icsd_237739	Au ₅ MnY ₃	148	148.17	0.00	Γ_1^+
icsd_079165	B ₂ MnO ₆ Sn	148	148.17	2.91	Γ_1^+
icsd_174290	Ba ₂ BiIrO ₆	148	2.4	0.20	$\Gamma_2^+\Gamma_3^+$
icsd_152678	Ba ₂ IrLaO ₆	148	2.4	0.49	$\Gamma_2^+\Gamma_3^+$
icsd_155549	Ba ₂ LaO ₆ Ru	148	148.17	1.29	Γ_1^+
icsd_419467	Ba ₆ N ₆ OOs ₂	148	2.4	0.00	$\Gamma_2^+\Gamma_3^+$
icsd_240981	BaF ₆ Ir	148	148.17	1.17	Γ_1^+
icsd_062157	BaMo ₆ S ₈	148	2.4	0.00	$\Gamma_2^+\Gamma_3^+$
icsd_076421	Br ₃ Fe	148	2.4	0.75	$\Gamma_2^+\Gamma_3^+$
icsd_039242	Br ₃ Ti	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 ₆ Rh	148	2.4	0.48	$\Gamma_2^+\Gamma_3^+$
icsd_670349	CaMnO ₃	148	148.17	1.64	Γ_1^+
icsd_033288	Cl ₂ CoO ₈	148	148.17	3.64	Γ_1^+
icsd_033289	Cl ₂ NiO ₈	148	2.4	3.18	$\Gamma_2^+\Gamma_3^+$
icsd_022081	Cl ₃ Cr	148	148.17	2.23	Γ_1^+
icsd_002552	Cl ₃ MnNa	148	148.17	4.16	Γ_1^+
icsd_038237	Cl ₃ V	148	2.4	1.75	$\Gamma_2^+\Gamma_3^+$
icsd_425145	Cl ₆ Re	148	148.17	0.00	Γ_1^+
icsd_025014	CoF ₆ Sn	148	148.17	3.67	Γ_1^+
icsd_016548	CoO ₃ Ti	148	2.4	3.07	$\Gamma_2^+\Gamma_3^+$
icsd_169192	CoO ₆ Pb ₂ Te	148	148.17	1.19	Γ_1^+
icsd_079268	Cr ₂ Ge ₂ Te ₆	148	148.17	0.01	Γ_1^+
icsd_071020	Cr ₂ Si ₂ Te ₆	148	148.17	0.09	Γ_1^+
icsd_010347	CrF ₆ Hg	148	148.17	0.52	Γ_1^+
icsd_418672	CrF ₆ K	148	2.4	0.93	$\Gamma_2^+\Gamma_3^+$
icsd_010344	CrF ₆ Mg	148	2.4	0.92	$\Gamma_2^+\Gamma_3^+$
icsd_418671	CrF ₆ Na	148	148.17	0.95	Γ_1^+
icsd_418673	CrF ₆ Rb	148	2.4	0.92	$\Gamma_2^+\Gamma_3^+$
icsd_251655	CrI ₃	148	148.17	0.63	Γ_1^+

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_626809	CrSiTe ₃	148	148.17	0.06	Γ_1^+
icsd_201511	CsF ₆ Re	148	148.17	0.32	Γ_1^+
icsd_025016	CuF ₆ Sn	148	148.17	1.67	Γ_1^+
icsd_030116	CuF ₆ Zr	148	148.17	3.55	Γ_1^+
icsd_025011	F ₆ FeSn	148	2.4	3.06	$\Gamma_2^+ \Gamma_3^+$
icsd_042163	F ₆ HgRh	148	2.4	0.40	$\Gamma_2^+ \Gamma_3^+$
icsd_095777	F ₆ IrLi	148	148.17	0.80	Γ_1^+
icsd_027664	F ₆ KOs	148	148.17	1.74	Γ_1^+
icsd_165215	F ₆ KRh	148	2.4	0.23	$\Gamma_2^+ \Gamma_3^+$
icsd_165206	F ₆ LiOs	148	148.17	1.64	Γ_1^+
icsd_165208	F ₆ LiPt	148	2.4	0.39	$\Gamma_2^+ \Gamma_3^+$
icsd_095776	F ₆ LiRh	148	148.17	0.13	Γ_1^+
icsd_165203	F ₆ LiRu	148	2.4	1.98	$\Gamma_2^+ \Gamma_3^+$
icsd_042159	F ₆ MgRh	148	2.4	0.39	$\Gamma_2^+ \Gamma_3^+$
icsd_025010	F ₆ MnSn	148	2.4	3.29	$\Gamma_2^+ \Gamma_3^+$
icsd_015108	F ₆ NiPb	148	2.4	1.83	$\Gamma_2^+ \Gamma_3^+$
icsd_025015	F ₆ NiSn	148	148.17	2.99	Γ_1^+
icsd_042161	F ₆ RhZn	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 ₆ S 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 ₆ O ₁₂ Re	148	2.4	0.04	$\Gamma_2^+ \Gamma_3^+$
icsd_061217	IrLi ₈ O ₆	148	2.4	0.85	$\Gamma_2^+ \Gamma_3^+$
icsd_641241	KMo ₆ S ₈	148	148.18	0.00	Γ_1^+
icsd_059175	KO ₈ S ₂ V	148	2.4	2.33	$\Gamma_2^+ \Gamma_3^+$
icsd_062156	Mo ₆ S ₈ Sr	148	148.17	0.00	Γ_1^+
icsd_262503	C ₆ Ag ₃ KMnN ₆	149	5.15	2.50	Γ_3
icsd_201056	C ₆ Au ₃ CoKN ₆	149	5.13	1.89	Γ_3
icsd_249724	C ₆ Au ₃ KN ₆ Ni	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 ₈ RbSe 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 ₄ Ni ₃ O ₉ Si 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 ₄ S 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 ₂ W	160	160.67	0.00	Γ_2
icsd_201396	CrS ₂ Tl	160	160.67	0.00	Γ_2
icsd_626736	CrSe ₂ Tl	160	8.32	0.00	Γ_3
icsd_033995	GaMo ₄ S ₈	160	8.32	0.28	Γ_3
icsd_036563	GaMo ₄ Se ₈	160	8.32	0.31	Γ_3
icsd_158199	GaS ₈ V ₄	160	8.32	0.01	Γ_3
icsd_195253	GaSe ₈ V ₄	160	8.32	0.00	Γ_3
icsd_069571	H ₆ F ₃ O ₃ V	160	8.34	2.74	Γ_3
icsd_001372	HCrO ₂	160	160.67	2.12	Γ_2
icsd_639980	In ₂ MnSe ₄	160	160.67	0.00	Γ_2
icsd_641335	KS ₂ Ti	160	8.32	0.26	Γ_3
icsd_644994	NaS ₂ V	160	8.32	0.41	Γ_3
icsd_077990	RbS ₂ Ti	160	8.32	0.00	Γ_3
icsd_043410	S ₂ Ta	160	8.34	0.00	Γ_3
icsd_024315	Se ₂ Ta	160	8.34	0.00	Γ_3
icsd_187684	NiO ₃ Pb	161	161.71	0.00	Γ_2
icsd_080350	As ₂ CoO ₆	162	162.77	2.74	Γ_2^+

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_080351	As ₂ MnO ₆	162	12.62	2.18	Γ_3^+
icsd_080349	As ₂ NiO ₆	162	12.58	2.80	Γ_3^+
icsd_187098	As ₂ O ₆ Pd	162	12.58	1.51	Γ_3^+
icsd_173552	C ₆ Ag ₃ FeN ₆	162	12.58	1.87	Γ_3^+
icsd_043292	Cl ₃ Zr	162	162.77	0.00	Γ_2^+
icsd_201755	F ₆ Li ₂ Nb	162	12.62	0.10	Γ_3^+
icsd_291234	MnO ₆ Sb ₂	162	12.62	1.35	Γ_3^+
icsd_073985	CaCrF ₆ Li	163	163.83	3.57	Γ_2^+
icsd_062035	Cl ₆ CrNa ₃	163	15.89	2.69	Γ_3^+
icsd_043278	AgFeTe ₂	164	164.89	0.00	Γ_2^+
icsd_609482	Al ₃ Tc ₂	164	164.89	0.00	Γ_2^+
icsd_423734	Ba ₂ Ni ₃	164	164.89	0.00	Γ_2^+
icsd_246280	Ba ₃ CaIr ₂ O ₉	164	164.89	0.00	Γ_2^+
icsd_150431	Ba ₃ CoNb ₂ O ₉	164	164.89	2.20	Γ_2^+
icsd_171479	Ba ₃ MnNb ₂ O ₉	164	164.89	1.65	Γ_2^+
icsd_240281	Ba ₃ NiO ₉ Ta ₂	164	12.58	3.55	Γ_3^+
icsd_429826	BaCoNa ₂ O ₈ V ₂	164	12.58	3.08	Γ_3^+
icsd_429827	BaFeNa ₂ O ₈ V ₂	164	12.62	2.37	Γ_3^+
icsd_429824	BaLi ₂ MnO ₈ V ₂	164	12.58	3.43	Γ_3^+
icsd_052364	Br ₂ Co	164	12.58	2.30	Γ_3^+
icsd_052365	Br ₂ Fe	164	12.62	2.39	Γ_3^+
icsd_060250	Br ₂ Mn	164	164.89	3.15	Γ_2^+
icsd_026078	Br ₂ Ti	164	164.89	0.00	Γ_2^+
icsd_246906	Br ₂ V	164	12.58	2.98	Γ_3^+
icsd_064831	Cl ₂ Fe	164	12.62	2.97	Γ_3^+
icsd_023177	Cl ₂ Ti	164	164.89	0.00	Γ_2^+
icsd_015901	Cl ₂ V	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 ₂ S 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 ₂ Tl	164	164.89	0.00	Γ_2^+
icsd_240956	Cs ₂ F ₆ Ir	164	12.62	1.21	Γ_3^+
icsd_072832	Cs ₂ F ₆ Nb	164	12.62	0.00	Γ_3^+
icsd_425912	Cs ₂ F ₆ Tc	164	164.89	3.11	Γ_2^+
icsd_260887	CsFeMo ₂ O ₈	164	12.58	2.59	Γ_3^+
icsd_202907	CsMo ₂ O ₈ V	164	12.62	1.77	Γ_3^+
icsd_095779	F ₆ IrK ₂	164	12.62	1.11	Γ_3^+
icsd_240955	F ₆ IrRb ₂	164	12.62	1.16	Γ_2^+
icsd_001528	F ₆ K ₂ Re	164	164.89	1.63	Γ_2^+
icsd_028779	F ₆ K ₂ Rh	164	12.62	0.47	Γ_3^+
icsd_425914	F ₆ K ₂ Tc	164	164.89	3.02	Γ_2^+
icsd_425915	F ₆ Na ₂ Tc	164	164.89	3.07	Γ_2^+
icsd_072831	F ₆ NbRb ₂	164	12.58	0.40	Γ_3^+
icsd_028780	F ₆ Rb ₂ Rh	164	12.62	0.53	Γ_3^+
icsd_425918	F ₆ Rb ₂ Tc	164	164.89	3.07	Γ_2^+
icsd_100706	FeGa ₂ S ₄	164	12.58	0.65	Γ_3^+
icsd_052369	FeI ₂	164	12.58	1.69	Γ_3^+
icsd_153864	FeKMo ₂ O ₈	164	12.62	2.44	Γ_3^+
icsd_632443	FeLi ₂ S ₂	164	12.62	1.99	Γ_3^+
icsd_245665	FeMo ₂ O ₈ Rb	164	12.62	2.30	Γ_3^+
icsd_059230	Ga ₂ NiS ₄	164	12.58	0.98	Γ_3^+
icsd_088940	H ₂ CoO ₂	164	12.58	2.89	Γ_3^+
icsd_023591	H ₂ MnO ₂	164	164.89	1.27	Γ_2^+
icsd_028101	H ₂ NiO ₂	164	164.89	2.90	Γ_2^+
icsd_240663	H ₆ Cl ₂ Cu ₃ MgO ₆	164	164.89	2.17	Γ_2^+
icsd_162099	H ₆ Cl ₂ Cu ₃ O ₆ Zn	164	164.89	2.37	Γ_2^+
icsd_033673	I ₂ Mn	164	164.89	2.23	Γ_2^+
icsd_246907	I ₂ V	164	12.58	2.67	Γ_3^+
icsd_100782	K ₃ O ₈ V ₃	164	12.62	1.69	Γ_3^+
icsd_037327	Li ₂ MnO ₂	164	164.89	2.55	Γ_2^+
icsd_071421	Li ₂ NiO ₂	164	164.89	3.24	Γ_2^+
icsd_200709	LiS ₂ Ti	164	12.58	0.00	Γ_3^+

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_016303	LiS ₂ V	164	12.62	0.54	Γ_3^+
icsd_044908	LiTe ₂ Ti	164	12.58	0.00	Γ_3^+
icsd_182700	N ₃ V ₂	164	164.89	0.00	Γ_2^+
icsd_644993	NaS ₂ V	164	12.58	0.00	Γ_3^+
icsd_042559	NiTe ₂	164	164.89	0.00	Γ_2^+
icsd_086519	S ₂ V	164	12.58	0.02	Γ_3^+
icsd_086520	Se ₂ V	164	12.62	0.00	Γ_3^+
icsd_603582	Te ₂ V	164	12.62	0.00	Γ_3^+
icsd_160574	Ag ₂ NiO 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 ₂ IrO ₆ Sr	166	166.101	0.37	Γ_2^+
icsd_407802	Ba ₂ MnO ₆ Te	166	12.58	1.35	Γ_3^+
icsd_009457	Ba ₃ Cr ₂ O ₈	166	166.101	0.48	Γ_2^+
icsd_010341	BaCrF ₆	166	166.101	0.93	Γ_2^+
icsd_035396	BaF ₆ Ni	166	12.62	0.30	Γ_3^+
icsd_006038	BaF ₆ Rh	166	166.101	0.30	Γ_2^+
icsd_425966	Bi ₂ MnTe ₄	166	166.101	0.05	Γ_2^+
icsd_020372	BiFeO ₃	166	166.101	0.00	Γ_2^+
icsd_067500	Br ₂ Mn	166	166.101	3.21	Γ_2^+
icsd_022106	Br ₂ Ni	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 ₂ Co	166	12.62	2.93	Γ_3^+
icsd_004059	Cl ₂ Fe	166	12.62	3.00	Γ_3^+
icsd_033752	Cl ₂ Mn	166	166.101	3.80	Γ_2^+
icsd_014208	Cl ₂ Ni	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 ₃ In ₂ S ₂	166	12.58	0.00	Γ_3^+
icsd_005437	Co ₃ InS ₂ Sn	166	166.101	0.00	Γ_2^+
icsd_005435	Co ₃ S ₂ Sn 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 ₂ O ₆ Se ₂	166	12.58	3.77	Γ_3^+
icsd_006152	CoNaO ₂	166	12.58	1.31	Γ_3^+
icsd_031917	CoO ₂ Pd	166	12.62	0.00	Γ_3^+
icsd_031916	CoO ₂ Pt	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 ₆ Sr	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 ₂ Pd	166	12.58	0.00	Γ_3^+
icsd_671321	CRu ₂	166	166.101	0.00	Γ_2^+
icsd_028694	CsF ₆ Ru	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 ₃ Ti	166	166.101	1.40	Γ_2^+
icsd_028692	F ₆ KRu	166	12.58	1.92	Γ_3^+
icsd_061276	F ₆ MnRb ₂	166	12.58	4.38	Γ_3^+
icsd_030114	F ₆ NiSr	166	166.101	0.14	Γ_2^+
icsd_028693	F ₆ RbRu	166	12.58	2.01	Γ_3^+
icsd_042158	F ₆ RhSr	166	166.101	0.22	Γ_2^+
icsd_067701	Fe ₂ O ₄ Y	166	12.62	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)	Irrrep
icsd_000071	Fe ₃ Sn ₂	166	166.101	0.00	Γ_2^+
icsd_670405	Fe ₆ Ge ₄ Mg	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 ₂ Ni	166	166.101	0.61	Γ_2^+
icsd_108894	In ₂ Ni ₃ S ₂	166	12.58	0.00	Γ_3^+
icsd_640140	In ₂ Ni ₃ Se ₂	166	8.34	0.00	Γ_3^+
icsd_061692	IrKLi ₆ O ₆	166	166.101	0.61	Γ_2^+
icsd_071540	K ₂ MnO ₆ Se ₂	166	166.101	3.79	Γ_2^+
icsd_165117	K ₃ Mn ₂ O ₈	166	166.101	0.16	Γ_2^+
icsd_166489	KS ₂ Ti	166	12.58	0.70	Γ_3^+
icsd_641350	KS ₂ Zr	166	8.34	0.00	Γ_3^+
icsd_026608	LiNiO ₂	166	12.58	0.00	Γ_3^+
icsd_024594	LiO ₂ V	166	12.58	1.68	Γ_3^+
icsd_189825	LiS ₂ Ti	166	12.58	0.00	Γ_3^+
icsd_170347	NaO ₂ Ru	166	12.62	0.87	Γ_3^+
icsd_043439	NaO ₂ Ti	166	12.58	0.45	Γ_3^+
icsd_420137	NaO ₂ V	166	12.58	1.79	Γ_3^+
icsd_026305	NaS ₂ Ti	166	12.62	0.00	Γ_3^+
icsd_076541	NaS ₂ V	166	12.62	1.29	Γ_3^+
icsd_077597	NaSe ₂ V	166	12.62	0.67	Γ_3^+
icsd_108892	Ni ₃ Pb ₂ Se ₂	166	12.62	0.00	Γ_3^+
icsd_108893	Ni ₃ S ₂ Tl 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 ₃ NiO ₄	167	15.89	1.14	Γ_3^+
icsd_043311	BCrO ₃	167	15.85	2.13	Γ_3^+
icsd_045060	BO ₃ V	167	15.89	1.88	Γ_3^+
icsd_016675	F ₃ Pd	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 ₃ MnN ₃	176	11.54	0.00	$\Gamma_4^+ \Gamma_6^+$
icsd_053564	Fe ₃ Te ₃ Tl	176	11.54	0.00	$\Gamma_4^+ \Gamma_6^+$
icsd_100785	LaRu ₃ Si ₂	176	11.54	0.00	$\Gamma_4^+ \Gamma_6^+$
icsd_080772	MnN ₃ Sr ₃	176	176.143	0.00	Γ_1^+
icsd_650662	Ru ₃ Si ₂ Y	176	176.143	0.00	Γ_1^+
icsd_079629	Se ₄ Ti ₃	176	176.143	0.00	Γ_1^+
icsd_077371	Si ₂ V	180	180.171	0.00	Γ_2^+
icsd_096025	Si ₂ V	181	181.177	0.00	Γ_2^+
icsd_042542	CFe ₃	182	182.183	0.00	Γ_2^+
icsd_053016	CoNb ₃ S ₆	182	182.183	0.00	Γ_2^+
icsd_624304	CoNb ₃ Se ₆	182	20.34	0.00	Γ_6^+
icsd_626392	CrNb ₃ S ₆	182	20.34	0.00	Γ_6^+
icsd_626398	CrNb ₃ Se ₆	182	20.34	0.00	Γ_6^+
icsd_626633	CrS ₆ Ta ₃	182	20.34	0.00	Γ_6^+
icsd_626727	CrSe ₆ Ta ₃	182	20.34	0.00	Γ_6^+
icsd_104913	MnNb ₃ S ₆	182	182.183	0.00	Γ_2^+
icsd_643023	MnNb ₃ Se ₆	182	20.34	0.00	Γ_6^+
icsd_643472	MnS ₆ Ta ₃	182	20.34	0.00	Γ_6^+
icsd_645400	Nb ₃ Se ₆ V	182	20.34	0.00	Γ_6^+
icsd_651111	S ₆ Ta ₃ V	182	20.34	0.00	Γ_6^+
icsd_651970	Se ₆ Ta ₃ V	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 ₃ CsCu	186	36.174	1.35	Γ_6^+
icsd_024792	CrSe	186	194.270	0.00	Γ_2^+
icsd_060417	F ₆ K ₂ Mn	186	186.207	3.79	Γ_2^+
icsd_025578	F ₆ MnRb ₂	186	36.175	4.42	Γ_6^+
icsd_184928	MnN	186	186.207	0.00	Γ_2^+
icsd_039504	MnNa ₂ O ₄	186	186.207	0.51	Γ_2^+
icsd_649860	Pt ₃ Y 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 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_290439	N ₂ Os	187	187.213	0.00	Γ_2
icsd_290430	N ₂ Ta	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 ₃ LiSc	188	188.219	0.00	Γ_2
icsd_150575	Al ₂ CoZr ₆	189	38.191	0.00	Γ_6
icsd_402701	Al ₂ FeZr ₆	189	38.191	0.00	Γ_6
icsd_027140	Al ₈ FeMg ₃ Si ₆	189	189.225	0.00	Γ_4
icsd_096905	Al ₉ FeMg ₃ Si ₅	189	189.225	0.00	Γ_4
icsd_083932	As ₂ CoZr 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 ₂ CoHf ₆	189	38.189	0.00	Γ_6
icsd_240169	Bi ₂ CoY ₆	189	189.225	0.00	Γ_4
icsd_020876	CoGa ₂ Zr 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 ₂ S ₆ Ta ₉	189	38.191	0.00	Γ_6
icsd_631770	FeGa ₂ Hf ₆	189	38.191	0.00	Γ_6
icsd_631856	FeGa ₂ Zr ₆	189	38.191	0.00	Γ_6
icsd_023577	FeGeHf	189	38.191	0.00	Γ_6
icsd_096249	FeLu ₆ Sb ₂	189	38.191	0.00	Γ_6
icsd_096247	FeSb ₂ Sc ₆	189	38.191	0.00	Γ_6
icsd_096248	FeSb ₂ Y ₆	189	38.191	0.00	Γ_6
icsd_156949	FeSb ₂ Zr ₆	189	38.191	0.00	Γ_6
icsd_090081	FeSc ₆ Te ₂	189	38.191	0.00	Γ_6
icsd_082530	FeTe ₂ Zr 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 ₅ N ₃ Ni 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 ₂ Cr	191	65.486	0.00	Γ_6^+
icsd_613892	B ₂ Fe	191	191.240	0.00	Γ_2^+
icsd_044439	B ₂ LuRu ₃	191	65.486	0.00	Γ_6^+
icsd_043664	B ₂ Mn	191	191.240	0.00	Γ_2^+
icsd_044581	B ₂ Ru ₃ Y	191	65.486	0.00	Γ_6^+
icsd_030331	B ₂ V	191	65.486	0.00	Γ_6^+
icsd_036504	BCaNi ₄	191	191.240	0.00	Γ_2^+
icsd_613036	BCo ₃ FeY	191	191.240	0.00	Γ_2^+
icsd_051272	BCo ₄ Y	191	191.240	0.00	Γ_2^+
icsd_058745	Be ₁₂ Ti	191	191.240	0.00	Γ_2^+
icsd_601122	BFe ₄ Lu	191	65.486	0.00	Γ_6^+
icsd_054474	CaNi ₅	191	191.240	0.00	Γ_2^+
icsd_260251	Co ₂ In ₉ K	191	191.240	0.00	Γ_2^+
icsd_623103	Co ₃ Ga ₂ La	191	191.240	0.00	Γ_2^+
icsd_102458	Co ₃ Ga ₂ Y	191	65.486	0.00	Γ_6^+
icsd_623631	Co ₆ Ge ₆ Ti	191	191.240	0.00	Γ_2^+
icsd_055564	CoSn	191	191.240	0.00	Γ_2^+
icsd_053466	Fe ₆ Ge ₆ Hf	191	191.240	0.00	Γ_2^+
icsd_084189	Fe ₆ Ge ₆ Lu	191	191.240	0.00	Γ_2^+
icsd_041461	Fe ₆ Ge ₆ Mg	191	191.240	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_092176	Fe ₆ Ge ₆ Nb	191	191.240	0.00	Γ_2^+
icsd_092170	Fe ₆ Ge ₆ Sc	191	191.240	0.00	Γ_2^+
icsd_092172	Fe ₆ Ge ₆ Ti	191	191.240	0.00	Γ_2^+
icsd_092174	Fe ₆ Ge ₆ Zr	191	191.240	0.00	Γ_2^+
icsd_632480	Fe ₆ LuSn ₆	191	191.240	0.00	Γ_2^+
icsd_633457	Fe ₆ ScSn 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 ₆ Mn ₆ Zr	191	65.486	0.00	Γ_6^+
icsd_054930	HfMn ₆ Sn ₆	191	65.486	0.00	Γ_6^+
icsd_057416	LuMn ₆ Sn ₆	191	65.486	0.00	Γ_6^+
icsd_015995	Mn ₂ O ₃ Ta	191	65.486	0.00	Γ_6^+
icsd_054273	Mn ₆ ScSn ₆	191	65.486	0.00	Γ_6^+
icsd_054928	Mn ₆ Sn ₆ Zr	191	65.486	0.00	Γ_6^+
icsd_186421	N ₃ Ta ₂ Ti	191	65.486	0.00	Γ_6^+
icsd_181506	S ₂ Ti	191	191.240	0.00	Γ_2^+
icsd_613552	BCr ₅ Si ₃	193	63.464	0.00	Γ_6^+
icsd_173362	Bi ₅ La ₃ Mn	193	63.464	0.00	Γ_6^+
icsd_617535	CCr ₅ Si ₃	193	193.260	0.00	Γ_2^+
icsd_659155	CoLa ₅ Pb ₃	193	63.464	0.00	Γ_6^+
icsd_604209	CoPb ₃ Zr ₅	193	193.260	0.00	Γ_2^+
icsd_624928	CoSb ₃ Zr ₅	193	63.464	0.00	Γ_6^+
icsd_659152	CrLa ₅ Pb ₃	193	193.260	0.00	Γ_2^+
icsd_659154	FeLa ₅ Pb ₃	193	193.260	0.00	Γ_2^+
icsd_604198	FePb ₃ Zr ₅	193	63.464	0.00	Γ_6^+
icsd_104003	Ga ₃ Ti ₂ Zr ₃	193	63.464	0.00	Γ_6^+
icsd_103996	Ga ₃ Ti ₅	193	193.260	0.00	Γ_2^+
icsd_103997	Ga ₄ Ti ₅	193	193.260	0.00	Γ_2^+
icsd_076138	Ge ₃ Mn ₅	193	193.260	0.00	Γ_2^+
icsd_637143	Ge ₃ Mo ₅	193	193.260	0.00	Γ_2^+
icsd_638048	Ge ₃ Ti ₅	193	193.260	0.00	Γ_2^+
icsd_109145	I ₃ Nb	193	193.260	0.00	Γ_2^+
icsd_659153	La ₅ MnPb ₃	193	63.464	0.00	Γ_6^+
icsd_168592	La ₆ Mn ₂ S ₁₀	193	193.260	0.00	Γ_2^+
icsd_024359	Mn ₅ Si ₃	193	63.463	0.00	Γ_6^+
icsd_644410	Mo ₅ Si ₃	193	193.260	0.00	Γ_2^+
icsd_604200	NiPb ₃ Zr ₅	193	63.463	0.00	Γ_6^+
icsd_646460	NiSb ₃ Zr ₅	193	63.464	0.00	Γ_6^+
icsd_650598	RuSb ₃ Zr ₅	193	193.260	0.00	Γ_2^+
icsd_044386	Si ₃ Ti 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 ₃ CoLu 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 ₄ Fe	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 ₃ Rh	194	194.270	0.00	Γ_2^+
icsd_010486	BaSe ₃ V	194	194.270	0.00	Γ_2^+
icsd_058805	BiMn	194	194.270	0.00	Γ_2^+
icsd_027511	Cl ₃ CoCs	194	63.464	2.34	Γ_6^+
icsd_024305	Cl ₃ CoRb	194	63.463	2.22	Γ_6^+
icsd_108289	Co ₂ Ge	194	63.463	0.00	Γ_6^+
icsd_053018	Co ₃ Nb ₂ Si	194	63.464	0.00	Γ_6^+
icsd_009966	Co ₃ Sc ₂ Si	194	194.270	0.00	Γ_2^+
icsd_625031	Co ₃ Si	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 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_053090	CoTe	194	194.270	0.00	Γ_2^+
icsd_053124	Cr ₂ GaN	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 ₂ F ₆ Ni ₂	194	63.463	4.84	Γ_6^+
icsd_015092	CsF ₃ Ni	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 ₂ Ge	194	191.240	0.00	Γ_2^+
icsd_409622	Fe ₂ ILa ₂	194	63.464	0.00	Γ_6^+
icsd_103637	Fe ₂ Sn	194	194.270	0.00	Γ_2^+
icsd_631740	Fe ₃ Ga	194	63.463	0.00	Γ_6^+
icsd_023405	Fe ₃ Ge	194	194.270	0.00	Γ_2^+
icsd_053483	Fe ₃ GeZr ₂	194	63.463	0.00	Γ_6^+
icsd_053558	Fe ₃ SiZr ₂	194	63.464	0.00	Γ_6^+
icsd_024569	Fe ₃ Sn	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 ₃ Y	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 ₂ Ni ₃ Si	194	194.270	0.00	Γ_2^+
icsd_670879	Ni ₃ Sn	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 ₂ Ta	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 ₂ Re	205	61.436	0.00	Γ_4^+
icsd_251565	O ₂ Rh	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 ₃ Te ₄ V	215	111.255	0.19	Γ_5^+
icsd_189696	AlTi ₂	216	119.319	0.00	Γ_5^+

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_185882	AlTi ₂ Zn	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 ₂ HfSn	216	139.537	0.00	Γ_5
icsd_625319	Co ₂ SnZr	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 ₂ Sn	216	139.537	0.00	Γ_5
icsd_076099	MnPdSb	216	44.231	0.00	Γ_5
icsd_040908	MnPdTc	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 ₂ Si	216	160.67	0.00	Γ_5
icsd_191001	MnSc ₂ Sn	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 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_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 ₃ Ti	221	8.34	0.00	Γ_4^+
icsd_167812	Al ₃ V	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 ₃ Os	221	65.486	0.00	Γ_4^+
icsd_671086	BaO ₃ Tc	221	123.345	0.00	Γ_4^+
icsd_191203	BaO ₃ V	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 ₃ Tc	221	123.345	0.00	Γ_4^+
icsd_108129	CCo ₃ Sn	221	47.252	0.00	Γ_4^+
icsd_076797	CCo ₃ Zn	221	47.252	0.00	Γ_4^+
icsd_422858	CdCo ₃ N	221	10.46	0.00	Γ_4^+
icsd_033667	CdO ₃ Ti	221	123.345	0.00	Γ_4^+
icsd_023167	Cl ₃ MnTl	221	65.486	2.69	Γ_4^+
icsd_077154	CMn ₃ Zn	221	47.252	0.00	Γ_4^+
icsd_015246	CoF ₃ K	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 ₃ Sr	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 ₃ Pb	221	166.101	0.00	Γ_4^+
icsd_108903	CrO ₃ Sr	221	123.345	0.00	Γ_4^+
icsd_049583	CsF ₃ Fe	221	166.101	3.04	Γ_4^+
icsd_042930	CTi ₃ Tl	221	65.486	0.00	Γ_4^+
icsd_015424	F ₃ FeK	221	166.101	2.86	Γ_4^+
icsd_049586	F ₃ FeRb	221	166.101	2.90	Γ_4^+
icsd_015423	F ₃ KMn	221	65.486	2.60	Γ_4^+
icsd_015426	F ₃ KNi	221	166.101	3.70	Γ_4^+
icsd_073167	F ₃ KPd	221	65.486	0.35	Γ_4^+
icsd_028145	F ₃ KV	221	123.345	2.05	Γ_4^+
icsd_043722	F ₃ MnRb	221	123.345	2.93	Γ_4^+
icsd_030612	F ₃ Mo	221	65.486	1.12	Γ_4^+
icsd_060611	F ₃ NaV	221	166.101	0.27	Γ_4^+
icsd_025596	F ₃ Nb	221	123.345	0.00	Γ_4^+
icsd_671397	F ₃ NiRb	221	65.486	3.68	Γ_4^+
icsd_073166	F ₃ PdRb	221	65.486	0.43	Γ_4^+
icsd_028146	F ₃ RbV	221	123.345	2.47	Γ_4^+
icsd_030613	F ₃ Ta	221	166.101	0.00	Γ_4^+
icsd_077369	Fe ₁₁ Si ₅	221	123.345	0.00	Γ_4^+
icsd_103451	Fe ₃ Ga	221	65.486	0.00	Γ_4^+
icsd_053461	Fe ₃ Ge	221	166.101	0.00	Γ_4^+
icsd_103638	Fe ₃ Sn	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 ₃ Sr	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 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_168838	H ₂ Mg _{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 ₃ Sn	221	123.345	0.00	Γ_4^+
icsd_104732	La ₃ Tl	221	166.101	0.00	Γ_4^+
icsd_029119	LaMnO ₃	221	65.486	0.00	Γ_4^+
icsd_028908	LaO ₃ Ti	221	123.345	0.00	Γ_4^+
icsd_028925	LaO ₃ V	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 ₃ Sr	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 ₃ Sr	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 ₃ Tl	221	123.345	0.00	Γ_4^+
icsd_181144	NZr	221	166.101	0.00	Γ_4^+
icsd_187637	O ₃ PbV	221	123.345	0.00	Γ_4^+
icsd_187483	O ₃ RhSr	221	123.345	0.00	Γ_4^+
icsd_069360	O ₃ RuSr	221	166.101	0.00	Γ_4^+
icsd_109076	O ₃ SrTc	221	123.345	0.00	Γ_4^+
icsd_088982	O ₃ SrV	221	123.345	0.00	Γ_4^+
icsd_611501	AsTi ₃	223	167.107	0.00	Γ_4^+
icsd_638098	Ge ₃ V	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 ₂ Mn	225	166.101	0.00	Γ_4^+
icsd_057507	AlAu ₂ Ti	225	8.32	0.00	Γ_4^+
icsd_057607	AlCo ₂ Fe	225	139.537	0.00	Γ_4^+
icsd_057611	AlCo ₂ Hf	225	139.537	0.00	Γ_4^+
icsd_057618	AlCo ₂ Mn	225	166.101	0.00	Γ_4^+
icsd_057620	AlCo ₂ Nb	225	139.537	0.00	Γ_4^+
icsd_057634	AlCo ₂ Ta	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 ₂ Mn	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 ₂ V	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 ₂ InTi	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 ₂ FeGa	225	139.537	0.00	Γ_4^+
icsd_185936	Co ₂ FeGe	225	71.536	0.00	Γ_4^+
icsd_102392	Co ₂ FeIn	225	139.537	0.00	Γ_4^+
icsd_052958	Co ₂ FeSi	225	139.537	0.00	Γ_4^+
icsd_102438	Co ₂ GaMn	225	166.101	0.00	Γ_4^+
icsd_102441	Co ₂ GaNb	225	139.537	0.00	Γ_4^+
icsd_102451	Co ₂ GaTa	225	139.537	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_052971	Co ₂ GeMn	225	166.101	0.00	Γ_4^+
icsd_102483	Co ₂ HfSn	225	139.537	0.00	Γ_4^+
icsd_053002	Co ₂ MnSb	225	139.537	0.00	Γ_4^+
icsd_053007	Co ₂ MnSi	225	139.537	0.00	Γ_4^+
icsd_102531	Co ₂ MnSn	225	166.101	0.00	Γ_4^+
icsd_102554	Co ₂ NbSn	225	71.536	0.00	Γ_4^+
icsd_053086	Co ₂ SiV	225	166.101	0.00	Γ_4^+
icsd_102687	Co ₂ SnZr	225	139.537	0.00	Γ_4^+
icsd_623481	Co _{8.8} Ge ₄ Mn _{3.2}	225	139.537	0.00	Γ_4^+
icsd_151207	CoCu ₂ Sn	225	71.536	0.00	Γ_4^+
icsd_102385	CoFe ₂ Ga	225	166.101	0.00	Γ_4^+
icsd_052954	CoFe ₂ Ge	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 ₂ FeSn	225	166.101	0.00	Γ_4^+
icsd_102996	Cu ₂ InMn	225	166.101	0.00	Γ_4^+
icsd_054597	Cu ₂ InTi	225	166.101	0.00	Γ_4^+
icsd_053312	Cu ₂ MnSb	225	166.101	0.00	Γ_4^+
icsd_103057	Cu ₂ MnSn	225	166.101	0.00	Γ_4^+
icsd_061323	CuO	225	71.536	0.00	Γ_4^+
icsd_065410	F ₂ Ti	225	71.536	2.03	Γ_4^+
icsd_186065	Fe ₂ GeMn	225	166.101	0.00	Γ_4^+
icsd_186061	Fe ₂ MnSi	225	166.101	0.00	Γ_4^+
icsd_108436	Fe ₃ Ga	225	139.537	0.00	Γ_4^+
icsd_053462	Fe ₃ Ge	225	71.536	0.00	Γ_4^+
icsd_053545	Fe ₃ Si	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 ₂ Si	225	166.101	0.00	Γ_4^+
icsd_103615	FeRu ₂ Sn	225	166.101	0.00	Γ_4^+
icsd_670177	FeSi ₂	225	139.537	0.00	Γ_4^+
icsd_155336	Ga ₄ Mn ₄ Ni 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 ₂ V	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 ₂ Ti	225	166.101	0.00	Γ_4^+
icsd_056191	H ₂ V	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 ₂ Ti	225	139.537	0.00	Γ_4^+
icsd_104980	Mn ₂ SnW	225	166.101	0.00	Γ_4^+
icsd_236807	MnN	225	139.537	0.00	Γ_4^+
icsd_076080	MnNi ₂ Sb	225	166.101	0.00	Γ_4^+
icsd_104926	MnNi ₂ Sn	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 ₂ Sb	225	166.101	0.00	Γ_4^+
icsd_104945	MnPd ₂ Sn	225	139.537	0.00	Γ_4^+
icsd_104964	MnRh ₂ Sn	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 ₂ Si	225	139.537	0.00	Γ_4^+
icsd_191000	MnSc ₂ Sn	225	71.536	0.00	Γ_4^+
icsd_024251	MnSe	225	139.537	0.33	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_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 ₂ SbTi	225	225.117	0.00	Γ_4^+
icsd_105376	Ni ₂ SnV	225	139.537	0.00	Γ_4^+
icsd_009866	NiO	225	71.536	1.75	Γ_4^+
icsd_105327	NiRh ₂ Sn	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 ₂ SnV	225	166.101	0.00	Γ_4^+
icsd_424636	Ga ₄ Mn	229	166.101	0.00	Γ_4^+
icsd_027836	O ₄ Pt ₃	229	166.101	0.00	Γ_4^+

C. Collinear ferrimagnetic materials

The relevant information for ferrimagnetic materials is summarized in Table S32-S35, including their chemical formula, space group, magnetic space group, band gap and corresponding irreducible representations of crystallographic space group.

TABLE S32. 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 ₂ Cu ₃ O ₈	2	2.4	2.05	Γ_1^+
icsd_167202	CoFLiO ₄ S	2	2.4	3.41	Γ_1^+
icsd_050507	CrF ₆ Mo	2	2.4	0.62	Γ_1^+
icsd_193472	Cu ₃ Nb ₂ O ₈	2	2.4	0.20	Γ_1^+
icsd_001143	Cu ₃ O ₈ P ₂	2	2.4	2.07	Γ_1^+
icsd_050506	CuF ₆ Mo	2	2.4	0.70	Γ_1^+
icsd_079695	H ₂ As ₂ CuFe ₂ O 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 ₃ ClCu ₂ O ₃	11	11.54	1.70	Γ_2^+
icsd_624485	Co ₂ NiSe ₄	12	12.62	0.00	Γ_2^+
icsd_622499	CoCr ₂ S ₄	12	12.62	0.00	Γ_2^+
icsd_601038	CoCr ₂ Se ₄	12	12.62	0.00	Γ_2^+
icsd_622979	CoFe ₂ Se ₄	12	12.62	0.00	Γ_2^+
icsd_026173	CoMo ₂ S ₄	12	12.58	0.00	Γ_2^+
icsd_624874	CoS ₄ Ti ₂	12	12.62	0.00	Γ_2^+
icsd_624884	CoS ₄ V ₂	12	12.58	0.00	Γ_2^+
icsd_625002	CoSe ₄ Ti ₂	12	12.62	0.00	Γ_2^+
icsd_625012	CoSe ₄ V ₂	12	12.58	0.00	Γ_2^+
icsd_625931	Cr ₂ FeS ₄	12	12.62	0.27	Γ_2^+
icsd_043042	Cr ₂ FeSe ₄	12	12.62	0.00	Γ_2^+
icsd_016884	Cr ₂ NiS ₄	12	12.62	0.06	Γ_2^+
icsd_626655	CrS ₄ V ₂	12	12.58	0.00	Γ_2^+
icsd_633332	Fe _{0.5} S ₂ Ti	12	12.62	0.00	Γ_2^+
icsd_015043	Fe ₃ Se ₄	12	12.62	0.00	Γ_2^+
icsd_632972	FeNi ₂ Se ₄	12	12.62	0.00	Γ_2^+
icsd_603354	FeRh ₂ Se ₄	12	12.58	0.00	Γ_2^+
icsd_042563	FeS ₄ Ti ₂	12	12.62	0.00	Γ_2^+
icsd_035634	FeS ₄ V ₂	12	12.62	0.06	Γ_2^+
icsd_633504	FeSe ₄ Ti ₂	12	12.62	0.61	Γ_2^+
icsd_193869	Ni _{0.5} Se ₂ Ti	12	12.62	0.00	Γ_2^+
icsd_042558	Ni ₃ Se ₄	12	12.62	0.00	Γ_2^+
icsd_646388	NiS ₄ Ti ₂	12	12.62	0.00	Γ_2^+
icsd_035140	NiS ₄ V ₂	12	12.62	0.00	Γ_2^+
icsd_646544	NiSe ₄ Ti ₂	12	12.62	0.00	Γ_2^+
icsd_023970	NiSe ₄ V ₂	12	12.62	0.00	Γ_2^+
icsd_024566	S ₄ V ₃	12	12.62	0.00	Γ_2^+
icsd_601347	Se ₄ Ti ₃	12	12.58	0.00	Γ_2^+
icsd_043412	Te ₄ Ti ₃	12	12.58	0.00	Γ_2^+
icsd_041858	AsCoS	14	14.75	0.00	Γ_1^+
icsd_239671	Ca ₂ CrO ₆ Os	14	14.79	0.00	Γ_2^+
icsd_089955	Ca ₂ FeMoO ₆	14	14.75	0.67	Γ_1^+
icsd_238148	Ca ₂ FeO ₆ Os	14	14.75	0.72	Γ_1^+
icsd_181147	FeMn ₂ O ₆ Sb	14	14.79	1.53	Γ_2^+
icsd_096120	La ₂ NiO ₆ Ru	14	14.79	0.76	Γ_2^+
icsd_252567	Mn ₃ O ₆ Re	14	14.79	0.00	Γ_2^+
icsd_602022	HFeTi	17	51.296	0.00	Γ_3^-
icsd_632217	H ₂ FeTi	26	26.69	0.00	Γ_3^-
icsd_627741	Cu ₂ GeMnSe ₄	31	31.127	1.01	Γ_2^-
icsd_020082	AlB ₄ Cr ₃	47	47.252	0.00	Γ_4^+
icsd_171434	BaCo ₂ O ₅ Y	51	51.296	0.48	Γ_4^+
icsd_033996	CoCu ₂ O ₃	59	59.410	0.68	Γ_4^+
icsd_610884	AsMnNi	62	62.446	0.00	Γ_2^+
icsd_670822	CCo ₂ Fe	62	62.446	0.00	Γ_2^+
icsd_670825	CCrFe ₂	62	62.441	0.00	Γ_1^+
icsd_167127	CFe ₂ Ni	62	62.446	0.00	Γ_2^+
icsd_025726	Co ₂ P	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 ₃ Ti ₂	62	62.446	0.30	Γ_2^+

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_044188	B ₃ CoV	63	63.463	0.00	Γ_3^+
icsd_042629	CCr ₃ Ge	63	63.464	0.00	Γ_4^+
icsd_189439	Fe ₂ O ₃	63	63.464	0.59	Γ_4^+
icsd_065881	BaCu ₃ O ₄	65	65.485	1.22	Γ_2^+
icsd_050089	Cu ₆ O ₁₀ Sr ₄	65	65.485	0.00	Γ_2^+
icsd_044293	B ₄ Fe ₂ Mo	71	71.536	0.00	Γ_2^+
icsd_614748	B ₄ Mn ₂ Mo	71	71.536	0.00	Γ_2^+
icsd_670346	CaMnO ₃	71	71.536	0.13	Γ_3^+
icsd_416904	Cu ₃ O ₅ Sr ₂	71	71.536	0.37	Γ_3^+
icsd_150701	FeMoO ₆ Sr ₂	87	12.62	0.00	$\Gamma_3^+ \Gamma_4^+$
icsd_052332	Sb ₄ V ₅	87	12.62	0.00	$\Gamma_3^+ \Gamma_4^+$
icsd_042881	Te ₄ V ₅	87	12.62	0.00	$\Gamma_3^+ \Gamma_4^+$
icsd_067978	BaCuFeO ₅ Y	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 ₆ Fe ₂ Li	102	34.158	1.49	Γ_5^+
icsd_067711	Ba ₂ Fe ₃ O ₈ Y	123	47.252	0.00	Γ_5^+
icsd_015521	ClFe ₃ O ₈ Pb ₄	123	65.486	0.10	Γ_5^+
icsd_053505	FeNNi	123	65.486	0.00	Γ_5^+
icsd_613327	B ₂ Co ₅ Ta ₃	127	65.486	0.00	Γ_5^+
icsd_614755	B ₂ MnMo ₂	127	55.358	0.00	Γ_5^+
icsd_088317	B ₂ V ₃	127	65.486	0.00	Γ_5^+
icsd_059553	In ₄ Ti ₃	127	55.358	0.00	Γ_5^+
icsd_644412	Mo ₃ Si 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 ₃ Sr ₂ V	129	59.410	0.00	Γ_5^+
icsd_042329	AsMn ₂	129	129.417	0.00	Γ_3^+
icsd_042325	Mn ₂ Sb	129	129.417	0.00	Γ_3^+
icsd_200014	MoO ₆ Rh ₂	136	136.501	0.00	Γ_3^+
icsd_032011	As ₂ Ba ₂ Mn ₃ O ₂	139	139.537	0.00	Γ_3^+
icsd_032010	As ₂ Mn ₃ O ₂ Sr ₂	139	139.537	0.00	Γ_3^+
icsd_246541	Ba ₂ FeMoO ₆	139	139.537	0.00	Γ_3^+
icsd_032013	Ba ₂ Mn ₃ O ₂ Sb ₂	139	139.537	0.00	Γ_3^+
icsd_032014	Bi ₂ Mn ₃ O ₂ Sr ₂	139	139.537	0.00	Γ_3^+
icsd_617225	BiTi ₂	139	71.536	0.00	Γ_5^+
icsd_094079	FeMoO ₆ Sr ₂	139	139.537	0.00	Γ_3^+
icsd_084202	Mn ₃ N ₂	139	69.524	0.00	Γ_5^+
icsd_032012	Mn ₃ O ₂ Sb ₂ Sr ₂	139	139.537	0.00	Γ_3^+
icsd_188743	MoO ₆ OsPb ₂	139	139.537	0.00	Γ_3^+
icsd_188742	MoO ₆ OsSn ₂	139	139.537	0.00	Γ_3^+
icsd_246426	Bi ₂ CrFeO 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 ₃ Fe	150	5.13	0.00	Γ_3^+
icsd_029134	F ₃ Rh	150	5.15	0.00	Γ_3^+
icsd_155025	Fe ₂ In ₂ Se ₅	164	2.4	0.00	Γ_3^+
icsd_062661	Mn ₃ Nb ₆ O ₁₁	164	12.58	0.25	Γ_3^+
icsd_076020	O ₂ PTi ₃	164	164.89	0.00	Γ_2^+
icsd_670856	B ₄ Fe	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 ₂ P	189	38.191	0.00	Γ_6^+
icsd_643671	MnSiTi	189	189.225	0.00	Γ_4^+
icsd_614407	BGe ₃ V ₅	193	63.464	0.00	Γ_6^+
icsd_609885	CA ₃ V ₅	193	63.464	0.00	Γ_6^+
icsd_042585	Fe ₅ Si ₃	193	193.260	0.00	Γ_2^+
icsd_643689	Mn ₃ Si ₃ V ₂	193	193.260	0.00	Γ_2^+
icsd_182095	B ₄ Mo	194	63.463	0.00	Γ_6^+
icsd_624067	Co ₂ Mg	194	63.464	0.00	Γ_6^+

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_102673	Co ₂ Sn	194	194.270	0.00	Γ_2^+
icsd_189226	Co ₃ SiTi ₂	194	11.54	0.00	Γ_6^+
icsd_163332	Mn ₂ Sb	194	187.213	0.00	Γ_6^+
icsd_670785	AlCrHfV	216	160.67	1.06	Γ_5^2
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 ₂ Sb	216	44.231	0.00	Γ_5
icsd_671535	Mn ₂ Si	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	CaAlCo ₃	221	123.345	0.00	Γ_4^+
icsd_076790	CCo ₃ Mg	221	123.345	0.00	Γ_4^+
icsd_076793	CCo ₃ Sc	221	47.252	0.00	Γ_4^+
icsd_077152	CMgNi ₃	221	47.252	0.00	Γ_4^+
icsd_077394	CRu ₃ V	221	123.345	0.00	Γ_4^+
icsd_053506	Fe ₃ NPd	221	123.345	0.00	Γ_4^+
icsd_044864	Fe ₃ NPt	221	123.345	0.00	Γ_4^+
icsd_053502	Fe ₄ N	221	123.345	0.00	Γ_4^+
icsd_044369	Mn ₄ N	221	123.345	0.00	Γ_4^+
icsd_106087	SnTi ₃	221	123.345	0.00	Γ_4^+
icsd_057600	AlCo ₂ Cr	225	139.537	0.00	Γ_4^+
icsd_185966	AlCo ₂ Ti	225	139.537	0.00	Γ_4^+
icsd_057643	AlCo ₂ V	225	166.101	0.00	Γ_4^+
icsd_057654	AlCrFe ₂	225	139.537	0.00	Γ_4^+
icsd_057806	AlFe ₂ Mn	225	71.536	0.00	Γ_4^+
icsd_057807	AlFe ₂ Mo	225	166.101	0.00	Γ_4^+
icsd_057827	AlFe ₂ Ti	225	166.101	0.00	Γ_4^+
icsd_057832	AlFe ₂ V	225	166.101	0.00	Γ_4^+

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_057994	AlMn ₂ V	225	166.101	0.00	Γ_4^+
icsd_186059	AsFe ₂ Ti	225	166.101	0.00	Γ_4^+
icsd_102318	Co ₂ CrGa	225	139.537	0.00	Γ_4^+
icsd_416260	Co ₂ CrIn	225	139.537	0.00	Γ_4^+
icsd_102453	Co ₂ GaTi	225	139.537	0.00	Γ_4^+
icsd_102456	Co ₂ GaV	225	166.101	0.00	Γ_4^+
icsd_052989	Co ₂ GeTi	225	71.536	0.00	Γ_4^+
icsd_053080	Co ₂ SiTi	225	139.537	0.00	Γ_4^+
icsd_102682	Co ₂ SnTi	225	139.537	0.00	Γ_4^+
icsd_102684	Co ₂ SnV	225	166.101	0.00	Γ_4^+
icsd_102437	CoGa ₂ Mn	225	166.101	0.00	Γ_4^+
icsd_102755	CrFe ₂ Ga	225	139.537	0.00	Γ_4^+
icsd_185999	CrFe ₂ Sn	225	71.536	0.00	Γ_4^+
icsd_186721	Fe ₂ GaMn	225	166.101	0.00	Γ_4^+
icsd_103469	Fe ₂ GaTi	225	139.537	0.00	Γ_4^+
icsd_103473	Fe ₂ GaV	225	71.536	0.00	Γ_4^+
icsd_186056	Fe ₂ InTi	225	166.101	0.00	Γ_4^+
icsd_186060	Fe ₂ SbTi	225	71.536	0.00	Γ_4^+
icsd_053555	Fe ₂ SiV	225	166.101	0.00	Γ_4^+
icsd_103641	Fe ₂ SnTi	225	166.101	0.00	Γ_4^+
icsd_103644	Fe ₂ SnV	225	166.101	0.00	Γ_4^+
icsd_103813	GaMn ₂ V	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 ₂ V	225	166.101	0.00	Γ_4^+
icsd_076227	Mn ₃ Si	225	166.101	0.00	Γ_4^+
icsd_188333	Mn ₃ Sn	225	166.101	0.00	Γ_4^+
icsd_671341	Ru ₂ SbV	225	166.101	0.00	Γ_4^+

D. Noncollinear ferrimagnetic materials

The relevant information for noncollinear ferrimagnetic materials is summarized in Table S36-S37, including their chemical formula, space group, magnetic space group, band gap and corresponding irreducible representations of crystallographic space group.

TABLE S36. 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 ₄ Cu ₃ F ₁₀	2	1.1	3.20	Γ_1^-
icsd.416823	HCoO ₅ PZn	2	2.4	1.69	Γ_1^+
icsd.000902	AsClCo ₂ O ₄	11	11.50	3.38	Γ_1^+
icsd.415798	Cl ₂ Co ₂ O ₃ Te	11	11.50	2.74	Γ_1^+
icsd.657748	O ₂ Ti	11	2.4	0.00	Γ_2^+
icsd.088156	Ba ₂ IrLaO ₆	14	14.79	0.50	Γ_2^+
icsd.088158	Ba ₂ IrLuO ₆	14	14.79	0.27	Γ_2^+
icsd.088153	Ba ₂ IrO ₆ Sc	14	14.75	0.09	Γ_1^+
icsd.088155	Ba ₂ IrO ₆ Y	14	14.79	0.19	Γ_2^+
icsd.152444	Ca ₂ NiO ₆ Os	14	14.79	0.12	Γ_2^+
icsd.079495	CoIrLa ₂ O ₆	14	14.75	0.45	Γ_1^+
icsd.030410	CuO ₆ Sb ₂	14	14.79	1.28	Γ_2^+
icsd.165398	F ₄ Ru	14	14.75	1.55	Γ_1^+
icsd.006044	F ₆ Li ₂ Rh	14	14.75	0.47	Γ_1^+
icsd.195628	FeMn ₂ O ₆ Re	14	14.75	0.00	Γ_1^+
icsd.238316	InO ₆ OsSr ₂	14	14.79	1.02	Γ_2^+
icsd.414605	IrLa ₂ LiO ₆	14	14.79	0.36	Γ_2^+
icsd.079492	IrLa ₂ MgO ₆	14	14.79	0.59	Γ_2^+
icsd.413634	IrLa ₂ NaO ₆	14	14.79	0.47	Γ_2^+
icsd.079494	IrLa ₂ NiO ₆	14	14.75	0.52	Γ_1^+
icsd.075596	IrLa ₂ O ₆ Zn	14	14.79	0.50	Γ_2^+
icsd.088157	IrLuO ₆ Sr ₂	14	14.79	0.24	Γ_2^+
icsd.088152	IrO ₆ ScSr ₂	14	14.79	0.02	Γ_2^+
icsd.088154	IrO ₆ Sr ₂ Y	14	14.79	0.26	Γ_2^+
icsd.416199	La ₂ LiO ₆ Os	14	14.79	1.00	Γ_2^+
icsd.088522	La ₂ MgO ₆ Rh	14	14.75	0.00	Γ_1^+
icsd.088523	La ₂ O ₆ RhZn	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 ₃ O ₄	51	51.295	0.00	Γ_3^+
icsd.612536	B ₂ BaNi ₂	58	58.398	0.00	Γ_3^+
icsd.615019	B ₂ Ni ₂ Sr	58	14.75	0.00	Γ_4^+
icsd.406953	AsCoHf	62	62.446	0.00	Γ_2^+
icsd.193272	Bi ₃ Co	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 ₂ Fe	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 ₃ Sn ₂	62	62.447	0.00	Γ_3^+
icsd.636746	GeIrTi	62	62.446	0.00	Γ_2^+
icsd.196446	IrO ₃ Sr	62	62.448	0.07	Γ_4^+
icsd.075569	LaO ₃ Ru	62	62.447	0.61	Γ_3^+
icsd.056697	O ₃ RuSr	62	62.447	0.00	Γ_3^+
icsd.236435	CoO ₆ OsSr ₂	87	12.62	0.04	$\Gamma_3^+ \Gamma_4^+$
icsd.245819	CuO ₆ OsSr ₂	87	12.62	0.00	$\Gamma_3^+ \Gamma_4^+$
icsd.024563	S ₄ V ₅	87	12.62	0.00	$\Gamma_3^+ \Gamma_4^+$
icsd.652166	Se ₄ V ₅	87	12.62	0.33	$\Gamma_3^+ \Gamma_4^+$
icsd.023173	F ₆ Li ₂ Mo	94	18.19	1.13	Γ_5^+
icsd.025751	Cr ₃ GeN	113	18.19	0.00	Γ_5^+
icsd.030447	BCO ₂	121	72.544	0.00	Γ_5^+
icsd.160691	CCr ₂ LaSi 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 ₃ K	127	55.358	2.49	Γ_5^+
icsd.611100	As ₂ Ni ₄ Y	136	65.486	0.00	Γ_5^+
icsd.166673	CoO ₆ Ta ₂	136	58.398	3.01	Γ_5^+
icsd.418676	CrF ₆ Li ₂	136	58.398	1.01	Γ_5^+
icsd.424578	Cs ₃ NiO ₂	136	58.398	1.58	Γ_5^+
icsd.084789	CuO ₆ Sb ₂	136	58.398	1.30	Γ_5^+
icsd.074565	F ₆ Li ₂ Mo	136	58.398	1.20	Γ_5^+
icsd.095778	F ₆ Li ₂ Rh	136	58.398	0.47	Γ_5^+
icsd.040337	FeO ₆ Ta ₂	136	58.398	2.36	Γ_5^+

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_262579	K ₃ NiO ₂	136	58.398	1.58	Γ_5^+
icsd_424579	NiO ₂ Rb ₃	136	58.398	1.31	Γ_5^+
icsd_025775	CGeMn ₃	140	72.544	0.00	Γ_5^+
icsd_024651	Fe ₂ N	149	162.77	0.00	Γ_2^+
icsd_200999	Li ₂ O ₃ Re	161	9.37	0.37	Γ_3^+
icsd_044612	Fe ₂ N	162	162.77	0.00	Γ_2^+
icsd_041814	Sb ₂ V ₃	166	12.58	0.00	Γ_3^+
icsd_016673	F ₃ Ru	167	15.85	1.39	Γ_3^+
icsd_016649	F ₃ Ti	167	15.85	2.19	Γ_3^+
icsd_030624	F ₃ V	167	15.85	2.03	Γ_3^+
icsd_088670	BaCoO ₃	187	38.191	1.35	Γ_6^+
icsd_624869	Co ₂ S ₆ Ta 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 ₆ Ge ₆ Sc	191	191.239	0.00	Γ_3^+
icsd_658018	Cr ₆ Ge ₆ Y	191	191.239	0.00	Γ_3^+
icsd_029285	NP ₃ V ₅	193	193.258	0.00	Γ_4^+
icsd_016839	CoSi	198	19.27	0.00	Γ_4^+
icsd_166458	N ₂ Os	205	61.436	0.00	Γ_4^+
icsd_635637	Ga ₂ V ₃	213	155.45	0.00	Γ_5^+
icsd_052592	AgMn ₃ N	221	166.97	0.00	Γ_5^+
icsd_058547	AuNV ₃	221	12.58	0.00	Γ_5^+
icsd_043853	CaFe ₃	221	12.62	0.00	Γ_4^+
icsd_043860	CaMn ₃	221	12.58	0.00	Γ_5^+
icsd_076842	CFe ₃ Sn	221	166.101	0.00	Γ_4^+
icsd_076763	CFe ₃ Zn	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 ₃ Sn	221	12.58	0.00	Γ_5^+
icsd_247066	Co ₃ InN	221	10.46	0.00	Γ_4^+
icsd_053125	Cr ₃ GaN	221	166.97	0.00	Γ_5^+
icsd_053132	Cr ₃ IrN	221	166.101	0.00	Γ_4^+
icsd_053143	Cr ₃ NRh	221	166.101	0.00	Γ_4^+
icsd_053145	Cr ₃ NSn	221	12.58	0.00	Γ_5^+
icsd_053306	CuMn ₃ N	221	166.97	0.00	Γ_5^+
icsd_183372	CuNNi ₃	221	65.486	0.00	Γ_4^+
icsd_044865	Fe ₃ NNi	221	166.101	0.00	Γ_4^+
icsd_153274	Fe ₃ NRh	221	12.62	0.00	Γ_4^+
icsd_087399	GaMn ₃ N	221	12.58	0.00	Γ_5^+
icsd_097743	GeMn ₃	221	166.101	0.00	Γ_4^+
icsd_044659	IrMn ₃ N	221	65.486	0.00	Γ_4^+
icsd_076056	Mn ₃ NNi	221	166.101	0.00	Γ_4^+
icsd_076057	Mn ₃ NPd	221	166.101	0.00	Γ_4^+
icsd_076058	Mn ₃ NPt	221	166.101	0.00	Γ_4^+
icsd_076060	Mn ₃ NRh	221	166.101	0.00	Γ_4^+
icsd_076062	Mn ₃ NSn	221	166.101	0.00	Γ_4^+
icsd_076070	Mn ₃ NZn	221	166.97	0.00	Γ_5^+
icsd_096119	Mn ₃ Sb	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 S38-S47, including their chemical formula, space group, magnetic space group, band gap and corresponding irreducible representations of crystallographic space group.

TABLE S38. 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 ₂ Fe ₄ O 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 ₂ Co ₂ O ₅	2	2.6	3.62	Γ_1^-
icsd_246811	B ₂ Fe ₂ O ₅	2	2.6	3.24	Γ_1^-
icsd_006240	Ba ₂ CuO ₆ Te	2	2.6	1.41	Γ_1^-
icsd_059720	BiMnO ₅ V	2	2.6	2.48	Γ_1^-
icsd_418858	Br ₂ CoO ₃ Sb ₂	2	2.6	2.62	Γ_1^-
icsd_039784	Br ₃ Ti	2	2.6	2.27	Γ_1^-
icsd_410101	Cl ₇ MoOSe	2	2.6	1.78	Γ_1^-
icsd_196024	CMnO ₃	2	2.6	3.01	Γ_1^-
icsd_423336	Cs ₄ FeO ₃	2	2.6	1.37	Γ_1^-
icsd_240930	Cu ₂ Na ₂ O ₁₁ Si ₄	2	2.6	2.90	Γ_1^-
icsd_039439	CuMoO ₄	2	2.6	2.02	Γ_1^-
icsd_004189	CuO ₄ W	2	2.6	1.94	Γ_1^-
icsd_173748	F ₂ O ₇ Te ₂ V ₂	2	2.6	2.67	Γ_1^-
icsd_036208	Fe ₂ O ₇ P ₂	2	2.6	3.83	Γ_1^-
icsd_196300	FeSe	2	2.6	1.21	Γ_1^-
icsd_180390	FFeO ₄ S	2	2.4	2.30	Γ_1^+
icsd_180391	FLiNiO ₄ S	2	2.4	3.71	Γ_1^-
icsd_087710	H ₂ FeO ₅ V	2	2.6	2.49	Γ_1^-
icsd_167608	HFeLiO ₅ P	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 ₆ Si ₂ Ti	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 ₂ In ₅ Zr ₄	10	10.44	0.00	Γ_2^-
icsd_081569	Fe ₂ O ₁₂ Se ₄ Sr	10	10.42	2.33	Γ_1^+
icsd_601978	H ₂ FeTi	10	10.45	0.00	Γ_1^-
icsd_000901	AsClCu ₂ O ₄	11	11.54	1.38	Γ_2^-
icsd_162834	BiFeO ₃	11	11.55	0.00	Γ_2^-
icsd_411140	Cl ₇ CsTi ₂	11	11.52	2.68	Γ_2^-
icsd_065346	ClFeLiMoO ₄	11	11.52	2.67	Γ_2^-
icsd_001029	CoI ₄ Rb ₂	11	11.53	2.05	Γ_1^-
icsd_108896	CoO ₃ Sr	11	11.50	0.00	Γ_1^+
icsd_084825	CoPZr ₂	11	11.53	0.00	Γ_1^-
icsd_035044	Cr ₂ Nb ₂ Se ₁₀	11	11.52	0.00	Γ_2^-
icsd_166587	CsF ₅ NOOs	11	11.53	1.68	Γ_1^-
icsd_422751	CuNa ₂ O ₂	11	11.53	1.33	Γ_1^-
icsd_166586	F ₅ KNOOs	11	11.53	1.63	Γ_1^-
icsd_078042	F ₇ MnRbZr	11	11.53	4.76	Γ_1^-
icsd_078041	F ₇ MnTiZr	11	11.52	3.77	Γ_2^-
icsd_066513	FeTaTe ₃	11	11.52	0.00	Γ_2^-
icsd_187148	H ₄ Fe	11	11.53	0.00	Γ_1^-
icsd_075454	As ₂ Ba ₂ Mn ₂ O	12	12.61	1.02	Γ_1^-
icsd_043898	As ₂ Cr	12	12.60	0.00	Γ_2^-
icsd_611574	As ₂ V	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	BiMnSe ₂	12	12.62	0.92	Γ_2^+
icsd_423461	Br ₄ W	12	12.60	0.25	Γ_2^-
icsd_172782	BrMnS ₂ Sb	12	12.62	1.40	Γ_2^+
icsd_072389	Ca ₂ FeN ₂	12	12.61	0.94	Γ_1^-
icsd_096556	CaClFeO ₂	12	12.60	2.10	Γ_2^-
icsd_617825	CFe ₂ Si ₂ Y ₂	12	12.61	0.00	Γ_1^-
icsd_041802	Cl ₃ CrCs	12	12.62	1.02	Γ_2^+
icsd_002225	Cl ₃ CrRb	12	12.62	1.21	Γ_2^+
icsd_026108	Cl ₃ Mo	12	12.61	2.37	Γ_1^-
icsd_262639	Cl ₃ Tc	12	12.60	1.16	Γ_2^-
icsd_624616	Co ₂ P ₂ S ₆	12	12.60	1.91	Γ_2^-
icsd_290048	Fe ₂ LuO ₄	12	12.61	0.00	Γ_1^-
icsd_016252	Fe ₂ P ₂ S ₆	12	12.61	2.12	Γ_1^-

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_061392	FePS ₃	12	12.61	2.10	Γ_1^-
icsd_030011	FeS ₂ Tl	12	12.61	1.19	Γ_1^-
icsd_020661	FeSc ₂ Si ₂	12	12.61	0.00	Γ_1^-
icsd_100354	FeSe ₂ Tl	12	12.60	0.80	Γ_2^-
icsd_671146	H ₃ MgNi 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 ₂ P ₂ S 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 ₂ Pd ₂ S ₆	12	12.61	0.41	Γ_1^-
icsd_648076	P ₂ S ₆ V 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 ₃ V _{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 ₄ Re	13	13.68	0.80	Γ_1^-
icsd_067168	Cl ₇ CsTi ₂	13	13.67	2.77	Γ_2^-
icsd_063686	ClF ₆ O ₂ Ru	13	13.68	0.79	Γ_1^-
icsd_081061	CoMoO ₄	13	13.68	2.37	Γ_1^-
icsd_015851	CoO ₄ W	13	13.67	3.01	Γ_2^-
icsd_008128	FeNbO ₄	13	13.67	2.39	Γ_2^-
icsd_015192	FeO ₄ W	13	13.68	1.29	Γ_1^-
icsd_411172	K ₂ Mn ₃ S ₄	13	13.67	2.62	Γ_2^-
icsd_061078	MnMoO ₄	13	13.67	1.95	Γ_2^-
icsd_015850	MnO ₄ W	13	13.68	2.66	Γ_1^-
icsd_081060	MoNiO ₄	13	13.67	2.26	Γ_2^-
icsd_015852	NiO ₄ W	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 ₃ CrIn	14	14.78	1.28	Γ_1^-
icsd_190486	Ca ₂ InO ₆ Os	14	14.75	0.89	Γ_1^+
icsd_291608	Ca ₂ O ₆ OsSc	14	14.75	0.70	Γ_1^+
icsd_015590	Cl ₃ CuK	14	14.77	1.64	Γ_2^-
icsd_239557	Cl ₃ CuTl	14	14.77	1.10	Γ_2^-
icsd_004411	Cl ₃ MoO	14	14.77	1.81	Γ_2^-
icsd_074940	CoK ₂ O 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 ₆ Ta ₂	14	14.79	0.00	Γ_2^+
icsd_202451	CuO ₃ Te	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 ₂ Mn ₂ O ₃	14	14.78	1.47	Γ_1^-
icsd_023722	MoO ₂	14	14.77	0.00	Γ_2^-
icsd_173152	O ₂ Tc	14	14.77	0.30	Γ_2^-
icsd_015889	O ₂ V	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 ₃ V ₂	15	15.88	1.34	Γ_1^-
icsd_038315	P ₄ V	15	15.87	0.00	Γ_2^-
icsd_037026	FeNaS ₂	23	23.51	1.65	Γ_2^-
icsd_081204	Ca ₂ FeO ₆ W	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 ₂ Cu ₃ LaO ₇	47	47.253	0.00	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_161972	Ba ₂ Cu ₃ LuO ₇	47	47.253	0.00	Γ_1^-
icsd_041646	Ba ₂ Cu ₃ O ₇ Y	47	47.253	0.00	Γ_1^-
icsd_171433	BaCo ₂ O ₅ Y	47	47.251	0.00	Γ_4^-
icsd_164175	BaFe ₂ O ₅ Y	51	51.291	0.62	Γ_3^-
icsd_035130	Ca ₂ Mn ₂ O ₅	55	55.356	1.20	Γ_2^-
icsd_035219	CaMnO _{2.5}	55	55.356	0.90	Γ_2^-
icsd_073399	Cu ₂ La ₂ O ₅	55	55.359	0.69	Γ_1^-
icsd_077943	CuLaO _{2.5}	55	55.359	0.69	Γ_1^-
icsd_090183	Mn ₂ O ₅ Sr ₂	55	55.356	0.82	Γ_2^-
icsd_670573	CFe ₂	57	57.385	0.00	Γ_1^-
icsd_020933	Fe ₂ HfSi ₂	57	57.380	0.00	Γ_4^-
icsd_087157	Fe ₂ ScSi 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 ₂ N	58	58.399	0.00	Γ_1^-
icsd_165626	BaCrS ₂	59	59.407	0.17	Γ_4^-
icsd_428170	BaFe ₂ OS ₂	59	59.411	2.47	Γ_1^-
icsd_009422	Br ₃ Mo	59	59.407	2.00	Γ_3^-
icsd_028119	Br ₃ Ru	59	59.411	0.47	Γ_1^-
icsd_260162	Br ₃ Tc	59	59.407	0.59	Γ_3^-
icsd_080372	C ₂ CrSc	59	59.407	0.00	Γ_3^+
icsd_015094	CaCu ₂ O ₃	59	59.410	0.57	Γ_3^+
icsd_414041	Cl ₃ Ru	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 ₂ OS ₂ Sr	59	59.411	2.47	Γ_1^-
icsd_195027	Fe ₂ OSe ₂ Sr	59	59.411	2.36	Γ_1^-
icsd_173784	I ₃ Ti	59	59.407	1.51	Γ_4^-
icsd_074648	I ₃ Zr	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 ₃ Sn	59	59.411	0.00	Γ_1^-
icsd_009965	CV ₂	60	60.420	0.00	Γ_4^-
icsd_042979	Mn ₂ N	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 ₂ Fe	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 ₃ FeIn	62	62.443	1.83	Γ_3^-
icsd_036217	Br ₃ FeTl	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	CAIFe ₂	62	62.449	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_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 ₃ Tc	62	62.448	1.50	Γ_4^+
icsd_043521	CCo ₃	62	62.444	0.00	Γ_4^-
icsd_670826	CCu ₂ Fe	62	62.449	0.00	Γ_1^-
icsd_670834	CFe ₂ Ta	62	62.448	0.00	Γ_4^+
icsd_670836	CFe ₂ Ti	62	62.444	0.00	Γ_4^-
icsd_670839	CFe ₂ W	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 ₃ FeK	62	62.449	3.71	Γ_1^-
icsd_151925	ClMnS ₂ Sb	62	62.444	1.66	Γ_4^-
icsd_623417	Co ₂ Ge	62	62.449	0.00	Γ_1^-
icsd_044858	Co ₂ Si	62	62.449	0.00	Γ_1^-
icsd_165248	CoCrSi	62	62.449	0.00	Γ_1^-
icsd_004404	CoF ₃ Na	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 ₃ Y	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 ₂ LiO ₂	62	62.444	1.33	Γ_4^-
icsd_067558	Cu ₂ NaO 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 ₃ KPd	62	74.562	2.35	Γ_4^+
icsd_260758	Fe ₃ N	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 ₃ Tl	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 ₃ Ti	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 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_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 ₂ Sr	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 ₂ NiSr ₂	62	62.444	0.43	Γ_4^-
icsd_252431	NaO ₃ Os	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 ₂ Zr	63	63.465	0.00	Γ_1^-
icsd_195899	AsCo ₂ LaN	63	63.461	0.00	Γ_2^-
icsd_195898	AsFe ₂ LaN	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 ₃ Cr ₂	63	63.461	0.00	Γ_2^-
icsd_079258	B ₃ V 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 ₂ Cr ₂ V	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 ₂ La	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 ₃ Ti	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 ₂ O ₃ Sr	65	65.483	0.52	Γ_3^-
icsd_174209	F ₇ KTi ₂	65	65.487	2.51	Γ_1^-
icsd_261512	Fe ₂ O ₅ Sr ₃	65	65.484	0.00	Γ_2^-
icsd_009389	OTi ₂ Zr	65	65.483	0.00	Γ_3^-
icsd_186504	AsCaFFe	67	67.503	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_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 ₂ BaFe ₂	69	69.523	0.00	Γ_3^-
icsd_166017	As ₂ CaFe ₂	69	69.523	0.00	Γ_4^-
icsd_163208	As ₂ Fe ₂ Sr	69	69.523	0.00	Γ_3^-
icsd_044175	B ₄ Co ₂ Mo	71	71.535	0.00	Γ_3^-
icsd_067392	CoCs ₂ Se ₂	72	72.542	2.25	Γ_2^-
icsd_067387	CoK ₂ S ₂	72	72.542	2.72	Γ_2^-
icsd_067390	CoK ₂ Se ₂	72	72.542	2.34	Γ_2^-
icsd_067386	CoNa ₂ S ₂	72	72.542	2.45	Γ_2^-
icsd_624264	CoNa ₂ Se ₂	72	72.542	1.93	Γ_2^-
icsd_067388	CoRb ₂ S ₂	72	72.542	2.67	Γ_2^-
icsd_067391	CoRb ₂ Se ₂	72	72.542	2.32	Γ_2^-
icsd_065455	Cs ₂ MnS ₂	72	72.542	2.59	Γ_2^-
icsd_065458	Cs ₂ MnSe ₂	72	72.542	2.30	Γ_2^-
icsd_065461	Cs ₂ MnTe ₂	72	72.542	2.25	Γ_2^-
icsd_065453	K ₂ MnS ₂	72	72.542	2.67	Γ_2^-
icsd_069870	Ca ₂ ClFeO ₃	75	35.167	0.00	$\Gamma_3\Gamma_4$
icsd_103995	Ga ₃ Ti ₂	83	10.44	0.00	$\Gamma_3\Gamma_4$
icsd_056880	Ca ₂ ClFeO ₃	85	59.407	0.72	$\Gamma_3\Gamma_4$
icsd_024894	MoO ₅ P	85	85.62	1.88	Γ_1^-
icsd_027315	MoO ₅ V	85	85.62	2.23	Γ_1^-
icsd_613131	B ₄ Co ₄ La	86	13.67	0.00	$\Gamma_3\Gamma_4$
icsd_023081	BaFe ₂ S ₄	87	12.60	1.35	$\Gamma_3\Gamma_4$
icsd_238713	BaFe ₂ Se ₄	87	12.60	0.90	$\Gamma_3\Gamma_4$
icsd_086200	Ba ₂ CuHgO ₅ Tl	104	36.179	0.00	Γ_5^-
icsd_187030	AlTi	123	53.334	0.00	Γ_5^+
icsd_252344	As ₄ CaFe ₄ Rb	123	123.344	0.00	Γ_2^-
icsd_075725	Ba ₂ CaCu ₂ HgO ₆	123	123.347	0.00	Γ_1^-
icsd_064639	Ba ₂ Cu ₂ LaO ₈ Ta	123	123.347	0.00	Γ_1^-
icsd_098113	Ba ₂ Cu ₃ LuO ₆	123	123.347	0.00	Γ_1^-
icsd_153495	BaCo ₂ LaO ₆	123	65.483	0.00	Γ_5^-
icsd_171432	BaCo ₂ O ₅ Y	123	123.347	0.00	Γ_1^-
icsd_083690	BaMn ₂ O ₅ Y	123	123.347	0.00	Γ_1^-
icsd_107586	BiNi ₉ S ₈ Te	123	47.251	0.00	Γ_5^-
icsd_074165	CaCu ₂ O ₇ Sr ₂ Tl	123	123.347	0.00	Γ_1^+
icsd_168904	CaMnO ₃	123	63.466	0.00	Γ_5^+
icsd_074164	Cu ₂ O ₇ Sr ₂ TlY	123	123.347	0.00	Γ_1^+
icsd_168837	H ₂ Mg _{0.5} Ti _{0.5}	123	127.397	0.00	Γ_3^+
icsd_096951	KO ₅ S ₂ Ti ₂ Y ₂	123	123.347	0.00	Γ_1^-
icsd_009967	CoNb ₄ P	124	124.353	0.00	Γ_3^-
icsd_043233	CoNb ₄ Si	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 ₂ FeTa ₂	127	55.358	0.00	Γ_5^+
icsd_180529	As ₂ Cr ₂ Fe ₂ O ₆ Sr ₄	129	59.407	0.00	Γ_5^-
icsd_180528	As ₂ Fe ₂ O ₆ Sc ₂ Sr ₄	129	59.407	0.00	Γ_5^-
icsd_420654	AsBa ₂ FeO ₃ Sc	129	59.407	0.00	Γ_5^-
icsd_248365	AsBaFMn	129	59.407	1.22	Γ_5^-
icsd_420653	AsCrFeO ₃ Sr 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 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_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 ₂ O ₅ Y	129	129.419	0.25	Γ_1^-
icsd_015289	BaNiS ₂	129	59.407	0.00	Γ_5^-
icsd_010454	Bi ₂ CaMn	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 ₃ Sr ₂	129	67.503	0.83	Γ_5^-
icsd_096557	Ca ₂ ClFeO ₃	129	59.407	0.75	Γ_5^-
icsd_169992	Ca ₂ CuFeO ₃ S	129	59.407	0.63	Γ_5^-
icsd_169993	Ca ₂ CuFeO ₃ Se	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 ₃ Sr ₂	129	59.407	0.82	Γ_5^-
icsd_080798	ClFeO ₄ W	129	67.503	1.80	Γ_5^-
icsd_262357	Co ₂ O ₆ P ₂ Sc ₂ Sr 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 ₃ SSr ₂	129	59.407	1.31	Γ_5^-
icsd_191256	CrN ₂ Nb	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 ₃ SSr ₂	129	67.503	0.78	Γ_5^-
icsd_168586	Fe ₂ O ₆ P ₂ Sc ₂ Sr 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 ₃ Sr 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 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_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 ₄ In ₁₂	136	58.398	0.00	Γ_5^+
icsd_020314	Cr ₂ O ₆ W	136	136.502	0.99	Γ_4^-
icsd_015306	CrO ₆ Ta ₂	136	58.398	0.00	Γ_5^+
icsd_024795	Fe ₂ O ₆ Te	136	136.503	1.74	Γ_1^-
icsd_186045	Fe ₄ Ge ₂ Lu	136	58.395	0.00	Γ_5^-
icsd_186048	Fe ₄ Si ₂ Y	136	58.395	0.00	Γ_5^-
icsd_103447	FeGa ₃	136	58.395	0.00	Γ_5^-
icsd_002575	O ₆ V ₂ W	136	136.502	1.28	Γ_4^-
icsd_074985	B ₄ Mn ₄	138	67.503	0.00	Γ_5^-
icsd_609848	As ₂ BaCo ₂	139	71.535	0.00	Γ_5^-
icsd_166018	As ₂ BaFe ₂	139	69.523	0.00	Γ_5^-
icsd_609899	As ₂ CaCo ₂	139	71.535	0.00	Γ_5^-
icsd_610073	As ₂ Co ₂ La	139	69.523	0.00	Γ_5^-
icsd_610122	As ₂ Co ₂ Sr	139	71.535	0.00	Γ_5^-
icsd_074877	As ₂ CsFe ₂	139	139.536	0.00	Γ_2^-
icsd_163209	As ₂ Fe ₂ Sr	139	71.535	0.00	Γ_5^-
icsd_023653	B ₂ Co ₂ Y	139	71.535	0.00	Γ_5^-
icsd_252590	BaBi ₂ Mn ₂	139	71.535	0.00	Γ_5^-
icsd_010468	BaFe ₂ P ₂	139	69.523	0.00	Γ_5^-
icsd_000405	BaMn ₂ Sn ₂	139	139.536	0.00	Γ_2^-
icsd_000406	CaCo ₂ Ge ₂	139	71.535	0.00	Γ_5^-
icsd_010462	CaCo ₂ P ₂	139	139.536	0.00	Γ_2^-
icsd_081748	Co ₂ Ge ₂ Y	139	69.523	0.00	Γ_5^-
icsd_100438	Co ₂ S ₂ Tl	139	139.536	0.00	Γ_2^-
icsd_624957	Co ₂ ScSi ₂	139	71.535	0.00	Γ_5^-
icsd_626238	Cr ₂ LuSi ₂	139	139.536	0.00	Γ_2^-
icsd_633666	Fe ₂ Si ₂ Zr	139	139.536	0.00	Γ_2^-
icsd_641273	KNi ₂ S ₂	139	139.536	0.00	Γ_2^-
icsd_424686	KNi ₂ Se ₂	139	139.536	0.00	Γ_2^-
icsd_646396	Ni ₂ S ₂ Tl	139	139.536	0.00	Γ_2^-
icsd_646550	Ni ₂ Se ₂ Tl	139	139.536	0.00	Γ_2^-
icsd_086811	CrSb ₂	140	140.543	0.00	Γ_3^-
icsd_042520	Sb ₂ Ti	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 ₂ Ti	141	141.556	0.66	Γ_2^-
icsd_250709	BaCo ₂ O ₈ P ₂	147	147.15	2.76	Γ_1^-
icsd_417824	C ₆ FeMn ₂ N ₆	147	147.15	3.77	Γ_1^-
icsd_417825	C ₆ Mn ₂ N ₆ Os	147	147.15	3.30	Γ_1^-
icsd_417823	C ₆ Mn ₂ N ₆ Ru	147	147.15	3.65	Γ_1^-
icsd_164936	CrLaO ₆ Te	147	15.87	0.88	$\Gamma_2^- \Gamma_3^-$
icsd_027014	As ₂ BaNi ₂ O 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 ₂ O ₈ P ₂	148	148.19	3.56	Γ_1^-
icsd_280167	BaNi ₂ O ₈ P 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 ₂ Li ₆ Mn ₂ N ₆	148	148.19	1.53	Γ_1^-
icsd_041539	Cl ₁₂ Zr ₆	148	148.19	0.17	Γ_1^-
icsd_027500	Cl ₃ Fe	148	148.19	2.11	Γ_1^-
icsd_038236	Cl ₃ Ti	148	2.6	2.24	$\Gamma_2^- \Gamma_3^-$
icsd_031854	CoMnO ₃	148	148.19	0.68	Γ_1^-
icsd_087943	F ₃ Ni	148	2.4	1.46	$\Gamma_2^+ \Gamma_3^+$
icsd_056890	Fe ₂ P ₂ Se ₆	148	2.6	1.98	$\Gamma_2^- \Gamma_3^-$
icsd_024790	FeO ₃ Ti	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 ₆ Cr ₂ N ₆	148	148.19	0.00	Γ_1^-
icsd_412874	Li ₆ Mn ₂ N ₆ Sr ₂	148	148.19	1.43	Γ_1^-
icsd_643237	Mn ₂ P ₂ Se ₆	148	2.6	1.67	$\Gamma_2^- \Gamma_3^-$
icsd_029203	MnO ₃ Sn	148	2.6	1.30	$\Gamma_2^- \Gamma_3^-$
icsd_044407	MnO ₃ Ti	148	2.6	2.91	$\Gamma_2^- \Gamma_3^-$

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_054140	MnPSe ₃	148	2.6	1.66	$\Gamma_2^- \Gamma_3^-$
icsd_015988	NiO ₃ Ti	148	2.6	2.82	$\Gamma_2^- \Gamma_3^-$
icsd_017009	OTi ₆	159	163.82	0.00	Γ_2^-
icsd_029035	Cl ₃ Ti	162	12.60	2.16	Γ_3^-
icsd_248351	O ₆ Ru ₂ Sr	162	162.75	1.10	Γ_2^-
icsd_032730	CaCoF ₆ Li	163	15.87	2.86	Γ_3^-
icsd_032732	CaF ₆ LiNi	163	15.88	2.34	Γ_3^-
icsd_032731	CdCoF ₆ Li	163	15.87	2.52	Γ_3^-
icsd_039428	Cl ₃ Ti	163	15.87	2.23	Γ_3^-
icsd_039817	Cl ₆ FeHf	163	163.81	3.04	Γ_2^-
icsd_039666	Cl ₆ FeZr	163	15.87	3.24	Γ_3^-
icsd_183024	Cl ₆ MoNa ₃	163	15.87	2.93	Γ_3^-
icsd_032733	F ₆ LiNiSr	163	15.88	2.34	Γ_3^-
icsd_020042	OTi ₆	163	162.76	0.00	Γ_1^-
icsd_041793	As ₂ Mn ₂ Sr	164	12.60	0.51	Γ_3^-
icsd_039512	As ₂ Mn ₂ Zn	164	12.60	0.00	Γ_3^-
icsd_429102	As ₅ La ₄ Mn ₂	164	12.61	0.00	Γ_3^-
icsd_152482	Ba ₃ CaO ₉ Ru ₂	164	164.88	1.33	Γ_1^-
icsd_041791	Bi ₂ CaMn ₂	164	12.60	0.16	Γ_3^-
icsd_041789	CaMn ₂ Sb ₂	164	12.60	0.39	Γ_3^-
icsd_022074	Cl ₉ Cs ₃ Fe ₂	164	164.88	0.81	Γ_1^-
icsd_631804	Fe ₂ Ga ₂ S ₅	164	12.60	0.72	Γ_3^-
icsd_159909	Fe ₂ K ₃ NaO ₈	164	12.60	1.77	Γ_3^-
icsd_200009	Fe ₂ NaO ₃	164	164.88	0.00	Γ_1^-
icsd_634664	Ga ₂ Mn ₂ S ₅	164	164.88	0.47	Γ_1^-
icsd_416040	K ₃ NaO ₈ Ru ₂	164	12.60	1.26	Γ_3^-
icsd_073874	Li ₂ NiO ₂	164	165.96	3.46	Γ_2^+
icsd_041790	Mn ₂ Sb ₂ Sr	164	12.61	0.34	Γ_3^-
icsd_416038	NaO ₈ Rb ₃ Ru ₂	164	12.60	1.26	Γ_3^-
icsd_023574	OTi ₂	164	164.88	0.00	Γ_1^-
icsd_151457	AlO ₄ V ₂	166	12.58	0.00	Γ_3^+
icsd_025005	Ba ₂ NiO ₆ Te	166	166.100	2.85	Γ_1^-
icsd_280045	Ba ₃ Mn ₂ O ₈	166	12.60	1.81	Γ_3^-
icsd_085055	Cr ₂ O ₈ Sr ₃	166	166.100	0.61	Γ_1^-
icsd_078928	Cs ₄ F ₁₂ Fe ₂ KLi	166	12.60	3.96	Γ_3^-
icsd_157323	Fe ₂ InO ₄	166	166.100	0.00	Γ_1^-
icsd_041381	Fe ₆ Ge ₄ Li	166	166.100	0.00	Γ_1^-
icsd_029011	FeO ₂ Tl	166	166.100	1.11	Γ_1^-
icsd_099369	CoLaO ₃	167	15.85	1.51	Γ_3^+
icsd_025781	Cr ₂ O ₃	167	167.106	2.47	Γ_1^-
icsd_026629	F ₃ Mo	167	15.85	2.88	Γ_3^+
icsd_001473	O ₃ V ₂	167	15.88	1.04	Γ_3^-
icsd_036502	Ba ₃ FeN ₃	176	11.53	0.00	$\Gamma_3^- \Gamma_5^-$
icsd_095740	CBaF ₂ MnO ₃	176	176.145	4.29	Γ_2^-
icsd_057518	Al ₉ BaFe ₂	191	191.236	0.00	Γ_3^-
icsd_623434	Co ₆ Ge ₆ Hf	191	191.241	0.00	Γ_1^-
icsd_041459	Co ₆ Ge ₆ Li	191	191.241	0.00	Γ_1^-
icsd_623474	Co ₆ Ge ₆ Lu	191	191.241	0.00	Γ_1^-
icsd_415256	Co ₆ Ge ₆ Mg	191	191.241	0.00	Γ_1^-
icsd_623581	Co ₆ Ge ₆ Sc	191	191.241	0.00	Γ_1^-
icsd_041460	Co ₆ Ge ₆ Zr	191	191.241	0.00	Γ_1^-
icsd_191489	BSi ₃ V ₅	193	193.257	0.00	Γ_4^-
icsd_648274	P ₃ V ₅	193	63.461	0.00	Γ_5^-
icsd_172878	Ag ₃ Ni ₂ O ₄	194	63.461	0.00	Γ_5^-
icsd_261608	AgCoO ₂	194	63.461	0.00	Γ_5^-
icsd_181348	AlN ₃ V 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 ₄ Fe	194	194.266	0.00	Γ_3^-
icsd_016361	Ba ₂ Bi ₂ Mn ₂ O	194	194.271	0.06	Γ_1^-
icsd_016360	Ba ₂ Mn ₂ OSb ₂	194	194.271	0.34	Γ_1^-
icsd_058697	Be ₂ Cr	194	63.460	0.53	Γ_6^-
icsd_058714	Be ₂ Mn	194	63.461	0.00	Γ_5^-
icsd_058752	Be ₂ V	194	63.461	0.00	Γ_5^-
icsd_080373	C ₂ CrSc	194	194.266	0.00	Γ_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_042918	CaCr ₂	194	63.465	0.00	Γ_5^-
icsd_043874	CAsV ₂	194	63.461	0.00	Γ_5^-
icsd_076802	CCr ₂ Ge	194	63.461	0.00	Γ_5^-
icsd_183361	CCr ₂ Si	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 ₃ CsFe	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 ₃ GeMn 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 ₂ Ga ₂ S 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 ₂ Sn	194	63.463	0.00	Γ_6^+
icsd_157935	MnO ₃ Sr	194	63.459	1.82	Γ_6^-
icsd_290431	N ₂ Ta	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 ₂ Zr	225	166.100	0.00	Γ_5^-
icsd_057808	AlFe ₂ Ni	225	166.100	0.00	Γ_5^-
icsd_102433	Co ₂ GaHf	225	71.535	0.00	Γ_5^-
icsd_169731	Co ₂ GaNi	225	166.100	0.00	Γ_5^-
icsd_025324	Co ₂ GeLi	225	166.100	0.00	Γ_5^-
icsd_052994	Co ₂ GeZn	225	166.100	0.00	Γ_5^-
icsd_102646	Co ₂ ScSn	225	71.535	0.00	Γ_5^-
icsd_103460	Fe ₂ GaNi	225	139.536	0.00	Γ_5^-
icsd_186057	Fe ₂ GeTi	225	71.535	0.04	Γ_5^-

F. Noncollinear antiferromagnetic materials

The relevant information for noncollinear antiferromagnetic materials is summarized in Table S48-S49, including their chemical formula, space group, magnetic space group, band gap and corresponding irreducible representations of crystallographic space group.

TABLE S48. 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 ₃ S ₂ Sn ₂	12	12.58	0.00	Γ_1^+
icsd_186046	Fe ₄ Ge ₂ Lu	58	58.396	0.00	Γ_2^-
icsd_670828	CFeMn ₂	62	62.441	0.00	Γ_1^+
icsd_185418	MnO ₃ V	62	62.441	0.78	Γ_1^+
icsd_057009	C ₂ Cr ₃	63	63.465	0.00	Γ_1^-
icsd_609880	CAsCr ₃	63	63.465	0.00	Γ_1^-
icsd_291338	CCr ₃ P	63	63.459	0.00	Γ_3^-
icsd_291339	Cr ₃ NP	63	63.464	0.00	Γ_4^+
icsd_180767	Ni ₃ S ₂	63	63.459	0.00	Γ_3^-
icsd_644620	NPV ₃	63	63.465	0.00	Γ_1^-
icsd_055075	Se ₄ Ti ₅	87	87.79	0.01	Γ_2^-
icsd_015451	Te ₄ Ti 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 ₂ O ₆ Te	136	58.395	1.74	Γ_5^-
icsd_078778	CrF ₄	136	136.502	1.19	Γ_4^-
icsd_613152	B ₄ Co ₄ Lu	137	137.510	0.00	Γ_4^+
icsd_613410	B ₄ Co ₄ Y	137	137.510	0.00	Γ_4^+
icsd_025760	AsCr ₃ N	140	140.543	0.00	Γ_3^-
icsd_182435	Mn ₃ O ₆ Te	148	2.6	1.68	$\Gamma_2^- \Gamma_3^-$
icsd_016316	Mo ₃ Se ₄	148	1.1	0.00	Γ_1^-
icsd_020389	Fe ₃ N	149	182.181	0.00	Γ_1^-
icsd_025813	BaCoO ₂	152	5.13	2.11	Γ_3^-
icsd_004266	FeO ₄ P	152	152.35	2.69	Γ_2^-
icsd_010424	Ni ₃ S ₂	155	5.15	0.00	Γ_3^-
icsd_401027	Cl ₈ Na ₂ Ti ₃	160	8.32	1.85	Γ_3^-
icsd_036207	Fe ₃ O ₇ P	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 ₈ Mn ₃ Na ₂	166	166.101	4.28	Γ_2^+
icsd_401026	Cl ₈ Na ₂ Ti ₃	166	166.97	2.53	Γ_1^+
icsd_291388	Cs ₂ Cu ₃ F ₁₂ Sn	166	12.62	3.55	Γ_3^+
icsd_425834	H ₆ Cl ₂ Cu ₃ O ₆ Zn	166	12.62	2.25	Γ_3^+
icsd_024176	Ni ₃ Pb ₂ S ₂	166	166.97	0.00	Γ_1^+
icsd_100217	Ni ₃ S ₂ Sn ₂	166	12.58	0.00	Γ_3^+
icsd_094318	BLiMnO ₃	174	174.135	2.94	Γ_2^-
icsd_072920	S ₄ V ₃	176	11.53	0.00	$\Gamma_3^- \Gamma_5^-$
icsd_638088	Ge ₂ V	180	180.169	0.00	Γ_4^-
icsd_168997	FeO ₄ P	181	21.41	3.13	Γ_6^-
icsd_069692	Co ₆ LiP ₄	187	187.211	0.00	Γ_4^-
icsd_094412	Co ₆ MgP ₄	187	187.211	0.00	Γ_4^-
icsd_251064	Ag ₂ S ₆ TeV 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 ₂ P	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 ₂ Lu ₃ Mn ₃ Si	189	189.223	0.00	Γ_3^-
icsd_409925	GePdTi	189	38.189	0.00	Γ_6^-
icsd_410967	In ₃ Rh ₂ Ti 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 ₂ Co ₃ Hf	191	191.238	0.00	Γ_4^+
icsd_044171	B ₂ Co ₃ Lu	191	65.486	0.00	Γ_6^+
icsd_044179	B ₂ Co ₃ Sc	191	191.238	0.00	Γ_4^+
icsd_023655	B ₂ Co ₃ Y	191	191.238	0.00	Γ_4^+
icsd_044191	B ₂ Co ₃ Zr	191	191.238	0.00	Γ_4^+
icsd_089437	Ge ₆ Mn ₆ Sc	191	191.237	0.00	Γ_4^-
icsd_240144	Mn ₆ Sn ₆ Y	191	65.486	0.00	Γ_6^+

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_182148	Sn ₆ V ₆ Y	191	65.486	0.00	Γ_6^+
icsd_635612	Ga ₃ V ₅	193	193.259	0.00	Γ_3^+
icsd_044504	Ge ₃ V ₅	193	193.259	0.00	Γ_3^+
icsd_191487	Si ₃ V ₅	193	193.259	0.00	Γ_3^+
icsd_109292	Sn ₃ Ti 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 ₃ Sn	194	63.464	0.00	Γ_6^+
icsd_652343	SiTa ₂ V 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 ₂ Pd	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 ₂ Pd	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 ₃ NPd	221	166.97	0.00	Γ_5^+
icsd_053142	Cr ₃ NPt	221	166.101	0.00	Γ_4^+
icsd_168836	H ₂ Mg _{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 ₃ Ga	223	167.105	0.00	Γ_4^-
icsd_053127	Cr ₃ Ge	223	167.106	0.00	Γ_5^-
icsd_015904	Cr ₃ O	223	2.6	0.00	Γ_5^-
icsd_016835	Cr ₃ Si	223	167.106	0.00	Γ_5^-
icsd_104020	GaV ₃	223	167.106	0.00	Γ_5^-
icsd_611953	H ₃ AuTi 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 S50-S56, including their chemical formula, space group, magnetic space group, band gap and corresponding irreducible representations of crystallographic space group.

TABLE S50. 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 ₂ O ₆	4	4.9	2.16	Γ_2
icsd_020157	F ₆ FeNa ₃	4	4.7	3.94	Γ_1
icsd_008010	FeI ₄ Rb ₂	4	4.9	2.57	Γ_2
icsd_237487	FeLaNaO ₆ W	4	4.7	1.48	Γ_1
icsd_238786	K ₂ La ₂ Mn ₂ O ₁₂ W ₂	4	4.7	2.16	Γ_1
icsd_238788	K ₂ Mn ₂ O ₁₂ W ₂ Y ₂	4	4.9	2.39	Γ_2
icsd_238789	La ₂ Mn ₂ Na ₂ O ₁₂ W ₂	4	4.7	1.94	Γ_1
icsd_238785	La ₂ Mn ₂ O ₁₂ Rb ₂ W ₂	4	4.7	2.16	Γ_1
icsd_159097	LaMnNaO ₆ W	4	4.7	2.23	Γ_1
icsd_238791	Mn ₂ Na ₂ O ₁₂ W ₂ Y ₂	4	4.7	2.33	Γ_1
icsd_238793	Mn ₂ O ₁₂ Rb ₂ W ₂ Y ₂	4	4.9	2.42	Γ_2
icsd_084830	H ₂ BaCo ₂ O ₆ P ₂	5	5.13	3.78	Γ_1
icsd_425760	Ag ₂ FeS ₄ Si	7	7.26	2.04	Γ_2
icsd_039528	Br ₇ FeSe	7	7.24	1.91	Γ_1
icsd_200680	CoGeNa ₂ O ₄	7	7.24	2.46	Γ_1
icsd_238234	FeGeLi ₂ S ₄	7	7.26	2.23	Γ_2
icsd_238236	FeLi ₂ S ₄ Sn	7	7.26	2.30	Γ_2
icsd_281242	I ₆ K ₂ Re	7	7.24	0.67	Γ_1
icsd_429816	Li ₂ MnS ₄ Sn	7	7.24	2.25	Γ_1
icsd_192515	BiFeO ₃	9	9.39	2.09	Γ_2
icsd_010501	CoNa ₄ O ₃	9	9.39	1.89	Γ_2
icsd_069757	CuO	9	9.39	1.07	Γ_2
icsd_001410	FeNa ₄ O ₃	9	9.39	1.56	Γ_2
icsd_060759	CuF ₂ O ₃ W	11	11.50	2.68	Γ_1^+
icsd_252429	H ₃ ClCuO ₃ Zn	11	11.50	2.55	Γ_1^+
icsd_036582	HCuO ₅ SeTl	11	11.50	2.26	Γ_1^+
icsd_036581	HCuO ₅ STl	11	11.50	2.24	Γ_1^+
icsd_020453	AgF ₂	14	14.79	0.00	Γ_2^+
icsd_425149	AgF ₄ Na ₂	14	14.75	0.98	Γ_1^+
icsd_425100	B ₄ Mn	14	14.75	0.00	Γ_1^+
icsd_100793	Ba ₂ LaO ₆ Ru	14	14.79	1.34	Γ_2^+
icsd_190774	C ₂ NiO ₄	14	14.75	1.82	Γ_1^+
icsd_153001	Ca ₂ CoO ₆ Te	14	14.75	2.71	Γ_1^+
icsd_098732	Ca ₂ CoO ₆ W	14	14.75	2.50	Γ_1^+
icsd_083473	Ca ₂ FeO ₆ Sb	14	14.75	2.04	Γ_1^+
icsd_051615	Ca ₂ MnO ₆ W	14	14.75	1.94	Γ_1^+
icsd_098733	Ca ₂ NiO ₆ W	14	14.75	2.84	Γ_1^+
icsd_079451	CaIrO ₆ Sr ₂	14	14.75	0.22	Γ_1^+
icsd_250364	Cl ₄ V	14	14.75	1.43	Γ_1^+
icsd_411050	Cl ₆ Na ₃ Ti	14	14.75	2.71	Γ_1^+
icsd_202918	CoF ₄ Li	14	14.75	2.77	Γ_1^+
icsd_169193	CoO ₆ Pb ₂ Te	14	14.75	2.33	Γ_1^+
icsd_153002	CoO ₆ Sr ₂ Te	14	14.79	1.74	Γ_2^+
icsd_188476	Cr _{0.5} Mn _{0.5} O ₃ Y	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 ₄ Na ₂	14	14.75	3.85	Γ_1^+
icsd_065785	F ₄ V	14	14.79	2.81	Γ_2^+
icsd_172591	FeO ₆ Sr ₂ Ta	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 ₆ K ₂ Tc	14	14.75	1.09	Γ_1^+
icsd_097487	La ₂ LiO ₆ Ru	14	14.75	1.33	Γ_1^+
icsd_170175	La ₂ NaO ₆ Os	14	14.75	1.20	Γ_1^+
icsd_160372	La ₂ NaO ₆ Ru	14	14.75	1.52	Γ_1^+
icsd_073900	LaO ₃ V	14	14.75	1.78	Γ_1^+
icsd_202866	LuO ₆ RuSr ₂	14	14.75	1.29	Γ_1^+
icsd_097744	MnMoO ₆ Sr ₂	14	14.75	0.91	Γ_1^+
icsd_097745	MnO ₆ Sr ₂ W	14	14.75	1.62	Γ_1^+
icsd_193723	MnS ₂	14	14.75	0.00	Γ_1^+
icsd_095578	O ₃ VY	14	14.75	1.93	Γ_1^+
icsd_238311	O ₆ OsSr ₂ Y	14	14.79	0.81	Γ_2^+
icsd_049500	O ₆ RuSr ₂ Y	14	14.75	1.24	Γ_1^+
icsd_099370	CoLaO ₃	15	15.89	1.55	Γ_2^+

TABLE S51. Tabulated information on **altmagnetic** 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 ₆ Te	18	18.19	2.50	Γ_4^+
icsd_163978	MnMoO ₆ Te	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 ₂ O ₄	31	31.123	0.92	Γ_1^+
icsd_627355	Cu ₂ FeS ₄ Si	31	31.123	1.49	Γ_1^+
icsd_042490	Cu ₂ GeMnS ₄	31	31.127	0.92	Γ_2^+
icsd_193986	Cu ₂ MnS ₄ Si	31	31.125	2.26	Γ_4^+
icsd_628396	Cu ₂ MnSe ₄ Si	31	31.127	1.35	Γ_2^+
icsd_161306	FeLi ₂ O ₄ Si	31	31.123	2.48	Γ_1^+
icsd_071177	H ₂ KMnO ₅ P	31	31.125	3.73	Γ_4^+
icsd_087325	HFeO ₂	31	31.127	1.97	Γ_2^+
icsd_161305	Li ₂ MnO ₄ Si	31	31.125	3.34	Γ_4^+
icsd_670672	Li ₂ MnS ₄ Sn	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 ₃ Y	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 ₂ Si	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 ₂ O ₃	41	41.211	0.44	Γ_1^+
icsd_025754	CuGeO ₃	51	51.294	2.27	Γ_2^+
icsd_089669	CuO ₃ Si	51	51.294	2.57	Γ_2^+
icsd_670125	CuO ₂ Pt	53	53.326	0.59	Γ_2^+
icsd_009136	Cl ₄ MnNa ₂	55	55.358	4.18	Γ_4^+
icsd_400264	Cl ₄ Na ₂ Ti	55	55.353	2.55	Γ_1^+
icsd_022046	GeMn ₂ O ₄	55	55.358	1.91	Γ_4^+
icsd_041724	As ₂ Fe	58	58.393	0.00	Γ_1^+
icsd_196424	B ₄ Fe	58	58.398	0.00	Γ_4^+
icsd_194807	B ₄ Mn	58	58.393	0.00	Γ_1^+
icsd_419222	C ₂ H ₂ FeN ₄	58	58.393	3.07	Γ_1^+
icsd_034307	F ₂ Ni	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 ₄ O ₄ V 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 ₂ Ru	58	58.393	0.00	Γ_1^+
icsd_082689	CaO ₅ V ₂	59	59.410	2.13	Γ_3^+
icsd_015522	Cl ₃ CuRb	60	60.422	1.40	Γ_2^+
icsd_023382	CrCsI ₃	60	60.417	0.95	Γ_1^+
icsd_020365	F ₂ Mn	60	60.422	3.48	Γ_2^+
icsd_152811	Fe ₂ N	60	60.417	0.00	Γ_1^+
icsd_096077	Fe ₂ O 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 ₂ CoNb	62	62.441	0.00	Γ_1^+
icsd_613324	B ₂ CoTa	62	62.441	0.00	Γ_1^+
icsd_614129	BFe ₂ Ni	62	62.446	0.00	Γ_2^+
icsd_162895	BiFeO ₃	62	62.448	1.70	Γ_4^+
icsd_004064	Br ₃ FeK	62	62.441	3.16	Γ_1^+
icsd_075470	Br ₃ InMn	62	62.446	1.87	Γ_2^+
icsd_042441	Br ₃ KMn	62	62.446	3.53	Γ_2^+
icsd_035218	CaMnO ₃	62	62.447	0.53	Γ_3^+

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_172790	CaMoO ₃	62	62.447	0.01	Γ_3^+
icsd_051291	CaO ₃ Ru	62	62.441	0.50	Γ_1^+
icsd_081056	CaO ₃ V	62	62.448	0.81	Γ_4^+
icsd_670827	CCuFe ₂	62	62.447	0.00	Γ_3^+
icsd_670837	CFe ₂ V	62	62.448	0.00	Γ_4^+
icsd_032710	Cl ₃ KMn	62	62.441	4.29	Γ_1^+
icsd_023168	Cl ₃ MnTl	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 ₃ Se	62	62.441	3.15	Γ_1^+
icsd_000500	CoO ₃ Te	62	62.441	2.65	Γ_1^+
icsd_155834	CoO ₃ Y	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 ₃ Sc	62	62.441	2.36	Γ_1^+
icsd_238834	CrO ₃ Tl	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 ₃ FeNa	62	62.446	3.18	Γ_2^+
icsd_031820	F ₃ KMn	62	62.446	4.01	Γ_2^+
icsd_015621	F ₃ MnNa	62	62.446	3.74	Γ_2^+
icsd_009008	F ₃ NaNi	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 ₃ Tl	62	62.446	0.65	Γ_2^+
icsd_043260	FeO ₃ Y	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	FNbNbO ₂	62	62.447	0.00	Γ_3^+
icsd_084948	HMnO ₂	62	62.446	1.61	Γ_2^+
icsd_026420	I ₃ MnTl	62	62.446	1.96	Γ_2^+
icsd_008146	LaO ₃ Ti	62	62.441	1.42	Γ_1^+
icsd_063520	LaO ₃ V	62	62.446	1.70	Γ_2^+
icsd_185830	LuO ₃ V	62	62.448	1.55	Γ_4^+
icsd_055622	Mn ₃ Sn 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 ₃ Se	62	62.448	3.64	Γ_4^+
icsd_158732	MnO ₃ Ti	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 ₃ Se	62	62.446	2.84	Γ_2^+
icsd_646165	NiPTi	62	62.447	0.00	Γ_3^+
icsd_183450	O ₃ SrTc	62	62.441	1.61	Γ_1^+
icsd_095577	O ₃ VY	62	62.446	1.95	Γ_2^+
icsd_063228	BaS ₃ V	63	63.462	0.31	Γ_2^+
icsd_658704	Bi ₂ Cs ₂ Ni	63	63.457	0.24	Γ_1^+
icsd_161460	CCuN ₂	63	63.462	0.77	Γ_2^+
icsd_192148	CoF ₃ Na	63	63.464	3.96	Γ_4^+
icsd_251575	F ₃ FeNa	63	63.462	3.34	Γ_2^+
icsd_192141	F ₃ NaNi	63	63.462	4.90	Γ_2^+
icsd_180910	O ₃ RuSr	63	63.457	0.48	Γ_1^+
icsd_023265	Mn ₂ S ₄ Sn	65	65.486	0.90	Γ_3^+
icsd_670121	CuMgO ₂	67	67.506	1.29	Γ_3^+
icsd_670124	CuO ₂ Pb	74	74.558	1.08	Γ_2^+

TABLE S53. Tabulated information on **altmagnetic** 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)	Irrrep
icsd_174205	MoO ₃ Sr	74	74.554	0.00	Γ_1^+
icsd_183451	O ₃ SrTc	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 ₆ LiMnV	102	102.190	2.64	Γ_2^+
icsd_246244	CaFeO ₂	113	18.19	1.61	Γ_5^+
icsd_291413	MnMoO ₆ Te	113	18.19	2.76	Γ_5^+
icsd_063423	Ba ₂ Cu ₃ O ₆ Y	115	115.285	0.00	Γ_4^+
icsd_093241	CuSb ₃ Ti ₂	115	115.285	0.00	Γ_4^+
icsd_631756	FeGa ₃	118	34.158	0.00	Γ_5^+
icsd_192470	AgFe ₂ GaTe ₄	121	121.327	0.89	Γ_1^+
icsd_160047	CuFe ₂ InSe 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 ₂ V ₂	123	47.252	0.00	Γ_5^+
icsd_005431	B ₂ FeMo ₂	127	127.387	0.00	Γ_1^+
icsd_614047	B ₂ FeNb ₂	127	55.358	0.00	Γ_5^+
icsd_043016	B ₂ FeW ₂	127	127.387	0.00	Γ_1^+
icsd_107331	Co ₂ InZr ₂	127	127.391	0.00	Γ_2^+
icsd_004054	F ₃ KMn	127	55.358	3.98	Γ_5^+
icsd_085499	F ₄ FeRb	127	127.387	3.47	Γ_1^+
icsd_401730	In ₅ Ti 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 ₆ Ta ₂	136	136.499	1.17	Γ_2^+
icsd_009166	F ₂ Fe	136	58.398	3.26	Γ_5^+
icsd_009165	F ₂ Mn	136	136.499	3.59	Γ_2^+
icsd_009168	F ₂ Ni	136	65.486	4.43	Γ_5^+
icsd_016763	F ₂ Pd	136	58.398	1.77	Γ_5^+
icsd_032552	F ₂ V	136	58.398	2.68	Γ_5^+
icsd_165210	F ₆ Li ₂ Ru	136	136.499	1.46	Γ_2^+
icsd_201756	F ₆ Na ₂ Nb	136	65.486	0.09	Γ_5^+
icsd_633444	Fe ₄ ScSi ₂	136	136.495	0.00	Γ_1^+
icsd_168834	H ₂ Ti	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 ₂ Re	136	136.499	0.00	Γ_2^+
icsd_015071	O ₂ Ru	136	136.499	0.00	Γ_2^+
icsd_023600	O ₆ Ta ₂ V	136	136.499	0.45	Γ_2^+
icsd_092989	AsTiZr	139	71.536	0.00	Γ_5^+
icsd_186502	Fe ₂ Na ₂ OSe ₂	139	69.524	2.04	Γ_5^+
icsd_248378	BaIrO ₃	140	140.541	0.00	Γ_1^+
icsd_008000	CuF ₃ K	140	140.545	2.91	Γ_2^+
icsd_069656	CuF ₃ Rb	140	69.524	3.04	Γ_5^+
icsd_075412	F ₃ KMn	140	72.544	3.97	Γ_5^+
icsd_174206	MoO ₃ Sr	140	72.544	0.00	Γ_5^+
icsd_183452	O ₃ SrTc	140	140.541	1.66	Γ_1^+
icsd_613476	BCr	141	74.559	0.00	Γ_5^+
icsd_022093	Cl ₃ Ru	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 ₃ Os	161	161.69	0.29	Γ_1^+
icsd_073132	AlF ₆ LiPd	163	15.89	3.13	Γ_3^+
icsd_078748	F ₆ GaLiPd	163	15.89	3.02	Γ_3^+
icsd_075971	FeN ₂ W	163	194.268	0.05	Γ_1^+
icsd_034474	BFeO ₃	167	15.89	2.41	Γ_3^+
icsd_402039	BO ₃ Ti	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 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_015840	Fe ₂ O ₃	167	167.103	2.31	Γ_1^+
icsd_252432	LiO ₃ Os	167	167.103	0.28	Γ_1^+
icsd_001462	O ₃ Ti ₂	167	15.85	2.01	Γ_3^+
icsd_192733	BaCoO ₃	176	63.462	0.00	$\Gamma_3^+ \Gamma_5^+$
icsd_002769	BaFe ₂ O ₄	182	20.34	3.37	Γ_6^+
icsd_042687	FeNb ₃ S ₆	182	20.31	0.00	Γ_5^+
icsd_632811	FeNb ₃ Se ₆	182	20.31	0.00	Γ_5^+
icsd_633323	FeS ₆ Ta ₃	182	20.33	0.00	Γ_5^+
icsd_645098	Nb ₃ NiSe ₆	182	182.182	0.00	Γ_3^+
icsd_645331	Nb ₃ S ₆ Ti	182	20.33	0.21	Γ_5^+
icsd_645338	Nb ₃ S ₆ V	182	20.33	0.00	Γ_5^+
icsd_645394	Nb ₃ Se ₆ Ti	182	182.182	0.19	Γ_3^+
icsd_042650	NbS ₂ V _{0.333}	182	20.31	0.00	Γ_5^+
icsd_097539	Ba ₃ CrS ₅	185	36.176	0.00	Γ_5^+
icsd_022092	Cl ₃ Ru	185	185.200	0.39	Γ_4^+
icsd_023873	BaMnO ₃	186	194.268	1.35	Γ_3^+
icsd_002590	Br ₃ CrCs	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 ₃ CrCs	186	186.205	1.06	Γ_3^+
icsd_281495	ClFeN ₃ O 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 ₂ W	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 ₄ O ₈ Sr	187	187.211	0.00	Γ_4^+
icsd_022091	Cl ₃ Ru	188	40.206	0.36	Γ_5^+
icsd_413691	Br ₃ Ru	193	63.462	0.43	Γ_5^+
icsd_004068	Br ₃ Zr	193	63.462	0.91	Γ_5^+
icsd_240157	Ca ₅ MnPb ₃	193	193.259	0.00	Γ_3^+
icsd_022090	Cl ₃ Ru	193	193.259	0.38	Γ_3^+
icsd_026069	Cl ₃ Ti	193	193.259	2.51	Γ_3^+
icsd_023163	Cl ₃ Zr	193	63.457	1.14	Γ_5^+
icsd_633412	FeSb ₃ Zr ₅	193	193.259	0.00	Γ_3^+
icsd_023947	HfI ₃	193	193.259	0.03	Γ_3^+
icsd_023172	I ₃ Ti	193	63.462	1.66	Γ_5^+
icsd_023946	I ₃ Zr	193	63.462	0.54	Γ_5^+
icsd_080907	La ₃ Sb ₅ Ti	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 ₃ Ru	194	194.268	0.00	Γ_4^+
icsd_008193	BaS ₃ V	194	63.462	0.33	Γ_5^+
icsd_106318	Be ₂ Fe	194	63.462	0.00	Γ_5^+
icsd_616410	Be ₂ Ru	194	63.462	0.00	Γ_5^+
icsd_174041	Br ₃ CsFe	194	63.457	3.00	Γ_5^+
icsd_002782	Br ₃ CsMn	194	63.462	3.74	Γ_5^+
icsd_423829	Br ₃ CsNi	194	194.268	2.22	Γ_4^+
icsd_041320	Br ₃ CsTi	194	63.457	2.45	Γ_5^+
icsd_201829	Br ₃ CsV	194	63.462	3.28	Γ_5^+
icsd_009704	Br ₃ MnRb	194	194.268	3.45	Γ_4^+
icsd_015011	Br ₃ NiRb	194	194.268	2.20	Γ_4^+
icsd_154257	Br ₃ RbTi	194	63.457	2.45	Γ_5^+

TABLE S55. Tabulated information on **altmagnetic** 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 ₃ RbV	194	63.462	3.21	Γ_5^+
icsd_163549	C ₃ AlV 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 ₃ CoTi	194	63.462	3.16	Γ_5^+
icsd_036132	Cl ₃ CrCs	194	194.268	1.09	Γ_4^+
icsd_059371	Cl ₃ CsNi	194	194.268	3.00	Γ_4^+
icsd_049748	Cl ₃ CsTi	194	63.462	2.48	Γ_5^+
icsd_015932	Cl ₃ CsV	194	194.268	3.56	Γ_4^+
icsd_084212	Cl ₃ CuRb	194	194.268	1.17	Γ_4^+
icsd_015010	Cl ₃ NiRb	194	194.268	2.94	Γ_4^+
icsd_049747	Cl ₃ RbTi	194	63.462	2.47	Γ_5^+
icsd_201830	Cl ₃ RbV	194	63.462	3.50	Γ_5^+
icsd_249388	CN ₂ Ni	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 ₂ W	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 ₃ La	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 ₃ Mn	194	194.268	2.78	Γ_4^+
icsd_423830	CsI ₃ Ni	194	63.457	1.26	Γ_5^+
icsd_154258	CsI ₃ Ti	194	63.457	2.25	Γ_5^+
icsd_026453	CsI ₃ V	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 ₂ W	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 ₃ LaV	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 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_646897	NiTe ₂	205	61.436	0.00	Γ_4^+
icsd_066939	O ₂ Ru	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 [42–48]. Owing to the development of topological quantum chemistry and symmetry-indicator theory [49–53], tens of thousands of nonmagnetic topological materials have been identified [54–56]. 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 [57, 58]. Based on our magnetic structure database, we employ magnetic topological quantum chemistry to identify 1,070 magnetic topological materials [58, 59], 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. S3 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 QAHI), 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.

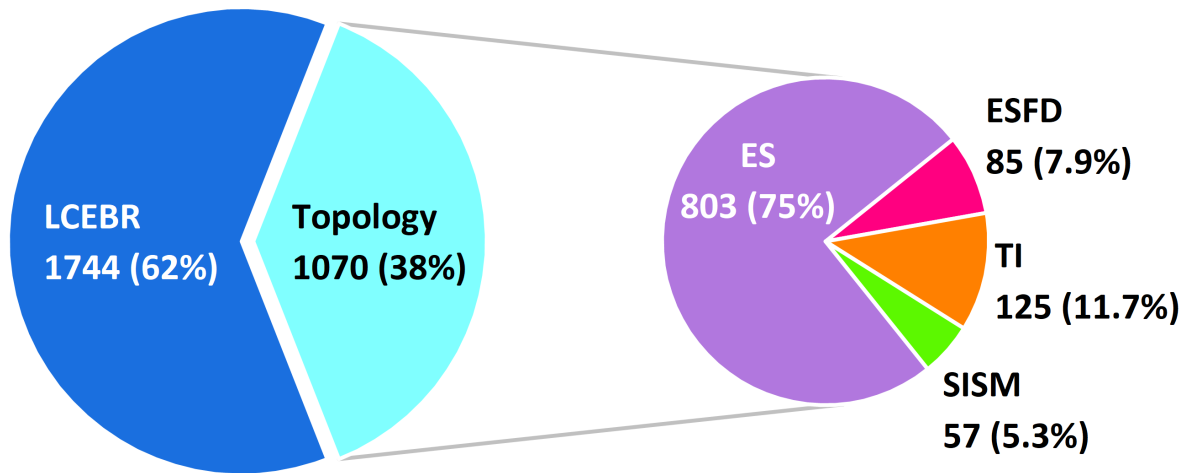


FIG. S3. Statistics of Topological Classification.

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) [60]. Its magnetic structure adopts a noncollinear AFM configuration, as illustrated in Fig. S4(a), corresponding to the magnetic space group $R32$ (155.45). As shown in Fig. S4(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. S4. 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) [61], which corresponds to the high-pressure structure of the altermagnet α - $MnTe$ [62, 63]. Under high pressure, α - $MnTe$ undergoes a structural phase transition from the NiAs-type to the MnP-type structure [61]. 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. S4(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. S4(e) and (f).

Co_3SnC (icsd_108129) crystallizes in the antiperovskite structure with space group $Pm\bar{3}m$ (No. 221) [64]. Its magnetic configuration is FM with magnetization oriented along the $[001]$ direction, as shown in Fig. S4(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. S4(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. S4(i).

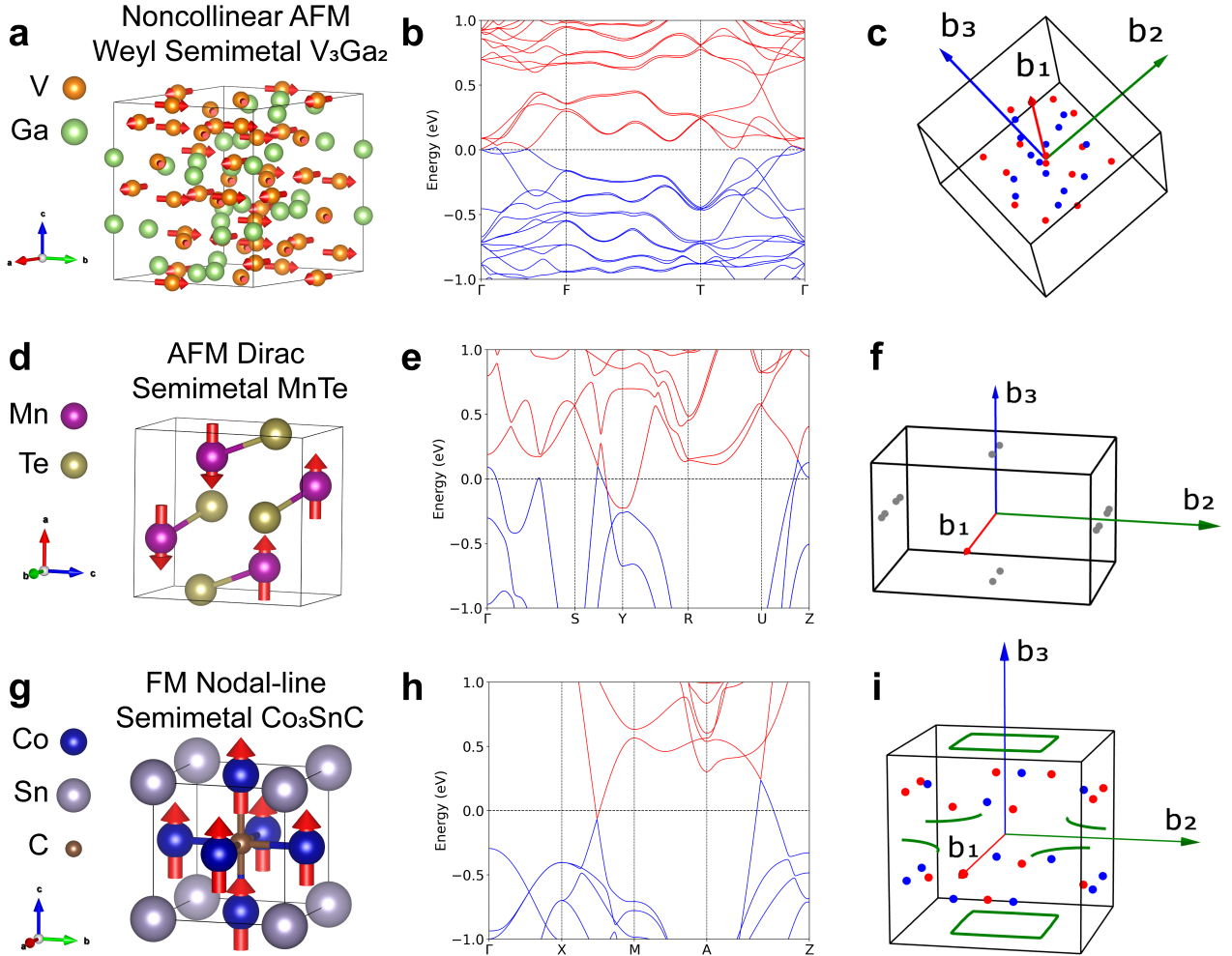


FIG. S4. Topological magnetic semimetals. (a)-(c) Magnetic structure, band structure, and distribution of Weyl points of the non-collinear AFM Weyl semimetal V_3Ga_2 . The magnetic moments of V lie in the xy plane, as indicated by red arrow. (d)-(f) Magnetic structure, band structure, and distribution 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. [58, 59]. The possible topological subclassifications include axion insulators (AXIs), three-dimensional quantum anomalous Hall insulators (3D QAHI), 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 S57. 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 ₄ Mn	12.62	$\eta_{4I} = 0; z_{2I,1} = 1; z_{2I,2} = 1$ $z_{2I,3} = 0$	3D QAHI
icsd.066509	Cu ₂ Li ₃ O 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 ₄ Si ₂	12.62	$\eta_{4I} = 2; z_{2I,1} = 1; z_{2I,2} = 1$ $z_{2I,3} = 0$	3D QAHI
icsd.169074	As ₂ BaOTi 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 ₃ Sr 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 ₂ P ₂	139.536	$z_2 = 1$	AXI
icsd.430064	Bi ₂ F ₂ OSr ₂ Ti 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 ₆ S ₈	2.4	$\eta_{4I} = 2; z_{2I,1} = 0; z_{2I,2} = 0$ $z_{2I,3} = 0$	AXI/3D QAHI
icsd.639106	HgMo ₆ S ₈	2.4	$\eta_{4I} = 2; z_{2I,1} = 0; z_{2I,2} = 0$ $z_{2I,3} = 0$	AXI/3D QAHI
icsd.641241	KMo ₆ S 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 ₂ N	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 ₂ V	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 ₃ S ₂ Sn ₂	12.62	$\eta_{4I} = 2; z_{2I,1} = 0; z_{2I,2} = 0$ $z_{2I,3} = 1$	3D QAHI
icsd.108894	In ₂ Ni ₃ S 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 ₂ MnTe 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 ₆ Ge ₄ Mg	166.101	$\eta_{4I} = 3; z_{2I,1} = 1; z_{2I,2} = 1$ $z_{2I,3} = 1$	3D QAHI
icsd.182148	Sn ₆ V ₆ Y	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 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_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 ₂ Ru	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 ₃ Sb	166.101	$\eta_{4I} = 2; z_{2I,1} = 1; z_{2I,2} = 1$ $z_{2I,3} = 1$	3D QAHI
icsd_168838	H ₂ Mg _{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 ₂ Cr	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 ₅ Sr ₂ Tl	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 ₄ Fe	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 ₂ P	11.54	$\eta_{4I} = 2; z_{2I,1} = 0; z_{2I,3} = 0$	AXI/3D QAHI
icsd_172559	Ag ₂ NiO 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 ₃ Cr ₂ Lu ₂	12.62	$\eta_{4I} = 0; z_{2I,1} = 0; z_{2I,2} = 0$ $z_{2I,3} = 1$	3D QAHI
icsd_617562	C ₃ Cr ₂ Y 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 ₂ Se 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 ₈ Lu 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 ₂ MnW ₂	55.358	$\eta_{4I} = 2$	AXI/3D QAHI

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_107331	Co ₂ InZr 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 ₂ FeNb ₂	55.358	$\eta_{4I} = 2$	AXI/3D QAHI
icsd_614207	B ₂ FeTa ₂	55.358	$\eta_{4I} = 2$	AXI/3D QAHI
icsd_062598	C ₂ CoSc	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 ₃ Nb	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 ₂ Pt	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 ₂ Pd	12.62	$\eta_{4I} = 2; z_{2I,1} = 0; z_{2I,2} = 0$ $z_{2I,3} = 0$	AXI/3D QAHI
icsd_160574	Ag ₂ NiO 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 ₅ La ₃ Mn	63.464	$\eta_{4I} = 0; z_{2I,1} = 1; z_{2I,2} = 1$ $\eta_{2I} = 0; z_{2R} = 1$	3D QAHI
icsd_053018	Co ₃ Nb ₂ Si	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 ₂ Se ₄	12.62	$\eta_{4I} = 2; z_{2I,1} = 1; z_{2I,2} = 1$ $z_{2I,3} = 1$	3D QAHI
icsd_023970	NiSe ₄ V ₂	12.62	$\eta_{4I} = 2; z_{2I,1} = 1; z_{2I,2} = 1$ $z_{2I,3} = 1$	3D QAHI
icsd_035140	NiS ₄ V ₂	12.62	$\eta_{4I} = 2; z_{2I,1} = 1; z_{2I,2} = 1$ $z_{2I,3} = 1$	3D QAHI
icsd_038369	Te ₂ V _{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 ₃ Se ₄	12.62	$\eta_{4I} = 2; z_{2I,1} = 1; z_{2I,2} = 1$ $z_{2I,3} = 0$	3D QAHI
icsd_042563	FeS ₄ Ti ₂	12.62	$\eta_{4I} = 2; z_{2I,1} = 1; z_{2I,2} = 1$ $z_{2I,3} = 0$	3D QAHI
icsd_603354	FeRh ₂ Se 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 ₂ Se ₄	12.62	$\eta_{4I} = 0; z_{2I,1} = 0; z_{2I,2} = 0$ $z_{2I,3} = 1$	3D QAHI
icsd_624485	Co ₂ NiSe ₄	12.62	$\eta_{4I} = 2; z_{2I,1} = 1; z_{2I,2} = 1$ $z_{2I,3} = 0$	3D QAHI
icsd_624874	CoS ₄ Ti ₂	12.62	$\eta_{4I} = 2; z_{2I,1} = 1; z_{2I,2} = 1$ $z_{2I,3} = 1$	3D QAHI
icsd_625002	CoSe ₄ Ti ₂	12.62	$\eta_{4I} = 2; z_{2I,1} = 1; z_{2I,2} = 1$ $z_{2I,3} = 1$	3D QAHI
icsd_626577	CrRh ₂ Se 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 ₂ Ti	12.62	$\eta_{4I} = 2; z_{2I,1} = 1; z_{2I,2} = 1$ $z_{2I,3} = 0$	3D QAHI
icsd_085291	Ba ₂ Cu ₃ LaO 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 ₂ Ni ₂ Sr	58.398	$\eta_{4I} = 2$	AXI/3D QAHI
icsd_044339	BCo ₃	62.446	$\eta_{4I} = 2$	AXI/3D QAHI
icsd_167127	CFe ₂ Ni	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 ₂ Fe	62.446	$\eta_{4I} = 2$	AXI/3D QAHI
icsd_670824	CCr ₂ Fe	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 ₄ V ₅	12.62	$\eta_{4I} = 2; z_{2I,1} = 0; z_{2I,2} = 0$ $z_{2I,3} = 0$	AXI/3D QAHI
icsd_614755	B ₂ MnMo ₂	55.358	$\eta_{4I} = 2$	AXI/3D QAHI
icsd_091199	CuMnO ₃ SSr 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 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_610777	As ₂ LaRh 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 ₃ AlV 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 ₃ NNi	166.101	$\eta_{4I} = 2; z_{2I,1} = 0; z_{2I,2} = 0$ $z_{2I,3} = 0$	AXI/3D QAHI
icsd_076060	Mn ₃ NRh	166.101	$\eta_{4I} = 2; z_{2I,1} = 0; z_{2I,2} = 0$ $z_{2I,3} = 0$	AXI/3D QAHI
icsd_052989	Co ₂ GeTi	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 ₂ V	166.101	$\eta_{4I} = 2; z_{2I,1} = 0; z_{2I,2} = 0$ $z_{2I,3} = 0$	AXI/3D QAHI
icsd_057994	AlMn ₂ V	166.101	$\eta_{4I} = 2; z_{2I,1} = 0; z_{2I,2} = 0$ $z_{2I,3} = 0$	AXI/3D QAHI
icsd_185936	Co ₂ FeGe	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. [58, 59].

TABLE S61. 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 ₄ S	11.54	$\eta_{4I} = 1; z_{2I,1} = 0; z_{2I,3} = 0$
icsd.099894	CoO ₃ Sr ₂	12.62	$\eta_{4I} = 3; z_{2I,1} = 0; z_{2I,2} = 0; z_{2I,3} = 0$
icsd.624999	CoSe ₄ Si 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 ₆ S ₈ Sr	148.17	$\eta_{4I} = 1; z_{2I,1} = 1; z_{2I,2} = 1; z_{2I,3} = 1$
icsd.237739	Au ₅ MnY ₃	148.17	$\eta_{4I} = 1; z_{2I,1} = 1; z_{2I,2} = 1; z_{2I,3} = 1$
icsd.075962	D ₁₂ Ba ₃ Ir ₂	12.62	$\eta_{4I} = 1; z_{2I,1} = 0; z_{2I,2} = 0; z_{2I,3} = 0$
icsd.079991	D ₈ BaFeMg ₂	12.62	$\eta_{4I} = 3; z_{2I,1} = 0; z_{2I,2} = 0; z_{2I,3} = 1$
icsd.086197	D ₂ CoO 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 ₃ S ₂ Sn ₂	166.101	$\eta_{4I} = 3; z_{2I,1} = 0; z_{2I,2} = 0; z_{2I,3} = 0$
icsd.053564	Fe ₃ Te ₃ Tl	11.54	$\eta_{4I} = 1; z_{2I,1} = 0; z_{2I,3} = 1$
icsd.080771	Ba ₃ MnN 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	ClMnMn ₃	166.101	$\eta_{4I} = 3; z_{2I,1} = 0; z_{2I,2} = 0; z_{2I,3} = 0$
icsd.160196	CrO ₃ Pb	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 ₂ Ti	166.101	$\eta_{4I} = 3; z_{2I,1} = 0; z_{2I,2} = 0; z_{2I,3} = 0$
icsd.096297	D ₂ Ti	166.101	$\eta_{4I} = 3; z_{2I,1} = 0; z_{2I,2} = 0; z_{2I,3} = 0$
icsd.424636	Ga ₄ Mn	166.101	$\eta_{4I} = 3; z_{2I,1} = 0; z_{2I,2} = 0; z_{2I,3} = 0$
icsd.611737	Au ₄ Cr	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 ₂ Se ₄ Ti	12.62	$\eta_{4I} = 1; z_{2I,1} = 1; z_{2I,2} = 1; z_{2I,3} = 0$
icsd.100785	LaRu ₃ Si ₂	11.54	$\eta_{4I} = 1; z_{2I,1} = 0; z_{2I,3} = 0$
icsd.040908	MnPdT _e	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 ₂ Mn	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 ₂ V	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 ₄ GaY ₄	12.62	$\eta_{4I} = 1; z_{2I,1} = 0; z_{2I,2} = 0; z_{2I,3} = 1$
icsd.084195	Se ₄ V ₃	12.62	$\eta_{4I} = 1; z_{2I,1} = 0; z_{2I,2} = 0; z_{2I,3} = 1$
icsd.201787	Mo ₂ S ₄ V	12.62	$\eta_{4I} = 1; z_{2I,1} = 0; z_{2I,2} = 0; z_{2I,3} = 1$
icsd.624816	CoRh ₂ Se ₄	12.62	$\eta_{4I} = 3; z_{2I,1} = 1; z_{2I,2} = 1; z_{2I,3} = 1$
icsd.632972	FeNi ₂ Se ₄	12.62	$\eta_{4I} = 1; z_{2I,1} = 0; z_{2I,2} = 0; z_{2I,3} = 1$

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_646388	NiS ₄ Ti ₂	12.62	$\eta_{4I} = 1; z_{2I,1} = 1; z_{2I,2} = 1; z_{2I,3} = 0$
icsd_646544	NiSe ₄ Ti ₂	12.62	$\eta_{4I} = 1; z_{2I,1} = 1; z_{2I,2} = 1; z_{2I,3} = 0$
icsd_095948	NiO ₃ Tl	14.79	$\eta_{4I} = 3; z_{2I,1} = 1$
icsd_239671	Ca ₂ CrO ₆ Os	14.79	$\eta_{4I} = 1; z_{2I,1} = 1$
icsd_031343	Li _{0.33} Se ₂ Ti	12.62	$\eta_{4I} = 1; z_{2I,1} = 0; z_{2I,2} = 0; z_{2I,3} = 1$
icsd_076020	O ₂ PTi 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 ₃ SiTi 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 ₂ GeMn	166.101	$\eta_{4I} = 3; z_{2I,1} = 0; z_{2I,2} = 0; z_{2I,3} = 0$
icsd_053312	Cu ₂ MnSb	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 ₂ Sb	166.101	$\eta_{4I} = 3; z_{2I,1} = 0; z_{2I,2} = 0; z_{2I,3} = 0$
icsd_103813	GaMn ₂ V	166.101	$\eta_{4I} = 1; z_{2I,1} = 0; z_{2I,2} = 0; z_{2I,3} = 0$
icsd_103892	GaNi ₂ V	166.101	$\eta_{4I} = 3; z_{2I,1} = 0; z_{2I,2} = 0; z_{2I,3} = 0$
icsd_188333	Mn ₃ Sn	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 S63. 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 ₃ MgNi ₂	12.61	icsd_613152	B ₄ Co ₄ Lu	137.51
icsd_074165	CaCu ₂ O ₇ Sr ₂ Tl	123.347	icsd_613410	B ₄ Co ₄ Y	137.51
icsd_252344	As ₄ CaFe ₄ Rb	123.344	icsd_023653	B ₂ Co ₂ Y	71.535
icsd_057651	AlCr ₂	71.535	icsd_052999	Co ₂ LaSi ₂	71.535
icsd_074877	As ₂ CsFe ₂	139.536	icsd_053088	Co ₂ Si ₂ Y	71.535
icsd_095837	CsMn ₂ P ₂	71.535	icsd_053491	Fe ₂ LaSi ₂	71.535
icsd_100438	Co ₂ S ₂ Tl	139.536	icsd_053556	Fe ₂ Si ₂ Y	71.535
icsd_167329	As ₂ Fe ₂ Rb	71.535	icsd_080506	Ge ₂ LaMn ₂	69.523
icsd_189036	As ₂ Fe ₂ K	71.535	icsd_081748	Co ₂ Ge ₂ Y	69.523
icsd_424686	KNi ₂ Se ₂	139.536	icsd_087581	Co ₂ LaP ₂	69.523
icsd_641273	KNi ₂ S ₂	139.536	icsd_610073	As ₂ Co ₂ La	69.523
icsd_646396	Ni ₂ S ₂ Tl	139.536	icsd_623465	Co ₂ Ge ₂ Lu	69.523
icsd_646550	Ni ₂ Se ₂ Tl	139.536	icsd_624957	Co ₂ ScSi ₂	71.535
icsd_658698	CsFe ₂ Sb ₂	69.523	icsd_632411	Fe ₂ LaP ₂	139.536
icsd_042529	BMn ₂	140.546	icsd_429102	As ₅ La ₄ Mn ₂	12.61
icsd_614745	B ₂ Mn	140.546	icsd_086369	MnScSi	189.223
icsd_067400	Cr ₂ N	12.61	icsd_099080	Ga ₂ Lu ₃ Mn ₃ Si	189.223
icsd_167802	NV ₂	12.6	icsd_643653	MnSiTa	189.224
icsd_024176	Ni ₃ Pb ₂ S ₂	166.97	icsd_023550	B ₂ Co ₃ Hf	191.238
icsd_041381	Fe ₆ Ge ₄ Li	166.1	icsd_044191	B ₂ Co ₃ Zr	191.238
icsd_157323	Fe ₂ InO ₄	166.1	icsd_079972	Ge ₆ LuMn ₆	65.483
icsd_041459	Co ₆ Ge ₆ Li	191.241	icsd_623474	Co ₆ Ge ₆ Lu	191.241
icsd_057518	Al ₉ BaFe ₂	191.236	icsd_623581	Co ₆ Ge ₆ Sc	191.241
icsd_658018	Cr ₆ Ge ₆ Y	191.239	icsd_624660	CoP ₂ W	194.268
icsd_187992	AlCo ₃	194.269	icsd_652343	SiTa ₂ V ₃	194.271
icsd_043860	CaMn ₃	166.97	icsd_102433	Co ₂ GaHf	71.535
icsd_044351	CGeMn ₃	166.97	icsd_102646	Co ₂ ScSn	71.535
icsd_077153	CMn ₃ Sn	166.97	icsd_065295	Cs ₄ Cu ₃ F ₁₀	2.6
icsd_015904	Cr ₃ O	167.106	icsd_079695	H ₂ As ₂ CuFe ₂ O ₁₀	2.6
icsd_016835	Cr ₃ Si	167.106	icsd_186046	Fe ₄ Ge ₂ Lu	58.396
icsd_053127	Cr ₃ Ge	167.106	icsd_615659	B ₄ V ₃	71.535
icsd_104020	GaV ₃	167.106	icsd_107586	BiNi ₉ S ₈ Te	47.251
icsd_025324	Co ₂ GeLi	166.1	icsd_169733	Co ₂ GaNi	71.535
icsd_016894	Co ₂ N	58.399	icsd_069692	Co ₆ LiP ₄	187.211
icsd_055578	Co ₂ In ₅ Zr ₄	10.44	icsd_094412	Co ₆ MgP ₄	187.211
icsd_171433	BaCo ₂ O ₅ Y	47.251	icsd_290889	FePTi	189.224
icsd_195900	AsLaNNi ₂	63.46	icsd_410967	In ₃ Rh ₂ Ti ₃	189.223
icsd_083690	BaMn ₂ O ₅ Y	123.347	icsd_610509	AsFeNi	189.223
icsd_096951	KO ₅ S ₂ Ti ₂ Y ₂	123.347	icsd_610530	AsFeTi	189.223
icsd_153495	BaCo ₂ LaO ₆	65.483	icsd_632938	FeNiP	189.223
icsd_171432	BaCo ₂ O ₅ Y	123.347	icsd_057808	AlFe ₂ Ni	166.1
icsd_186045	Fe ₄ Ge ₂ Lu	58.395	icsd_103460	Fe ₂ GaNi	139.536
icsd_633444	Fe ₄ ScSi 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 S64. 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 ₂ CsS ₂	69.524
icsd_050819	MnRbSe ₂	119.319	icsd_622533	Co ₂ CsSe ₂	69.524
icsd_087983	KMnTe ₂	119.319	icsd_623956	Co ₂ KS ₂	71.536
icsd_087984	MnRbTe ₂	119.319	icsd_624798	Co ₂ RbSe ₂	69.524
icsd_096699	CuO ₂	12.58	icsd_633338	Fe ₂ S ₂ Tl	139.537
icsd_160557	Ca ₂ CoO 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 ₃ RuSr	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 ₂ Sr	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 ₂ Ti ₂	47.252	icsd_069332	C ₃ D ₃ LaO ₆	160.67
icsd_430063	BaBi ₂ OTi ₂	47.252	icsd_187684	NiO ₃ Pb	161.71
icsd_430299	CsOS ₂ V ₂	47.252	icsd_200709	LiS ₂ Ti	12.58
icsd_634628	GaMn	47.252	icsd_609482	Al ₃ Tc ₂	164.89
icsd_104026	Ga ₅ V ₂	55.358	icsd_625401	CoTe ₂	12.58
icsd_249632	Ga ₅ Mn ₂	65.486	icsd_644993	NaS ₂ V	12.58
icsd_401730	In ₅ Ti ₂	127.391	icsd_005436	Co ₃ In ₂ S ₂	12.58
icsd_615683	B ₄ W	127.393	icsd_005437	Co ₃ InS ₂ Sn	166.101
icsd_015289	BaNiS ₂	59.407	icsd_023354	BrLa	12.58
icsd_042327	FeLiP	59.407	icsd_024410	CLa	12.58
icsd_042750	AlGeMn	129.417	icsd_026608	LiNiO ₂	12.58
icsd_107932	AsCoLi	129.417	icsd_100217	Ni ₃ S ₂ Sn ₂	12.58
icsd_162808	AsFFeSr	59.407	icsd_189825	LiS ₂ Ti	12.58
icsd_162902	CoSe	59.41	icsd_416314	Co _{1.5} SSn	12.58
icsd_237581	ClNiO ₃ Sr ₂	67.506	icsd_016675	F ₃ Pd	15.85
icsd_418853	CoGeMg	129.417	icsd_080772	MnN ₃ Sr ₃	176.143
icsd_428148	CaCoSi	129.416	icsd_650662	Ru ₃ Si ₂ Y	176.143
icsd_187715	NOs	131.441	icsd_077371	Si ₂ V	180.171
icsd_009423	CrO ₂	136.501	icsd_638088	Ge ₂ V	180.169
icsd_035382	F ₆ LiV ₂	136.501	icsd_096025	Si ₂ V	181.177
icsd_154021	O ₂ Re	136.499	icsd_042542	CFe ₃	182.183
icsd_026560	MnO ₄ Sr ₂	71.536	icsd_161882	Al _{0.75} NZr _{0.25}	186.207
icsd_055710	CuI ₂ O ₂ Sr ₂	71.536	icsd_168896	BTc	186.207
icsd_067362	Co ₂ Se ₂ Tl	69.524	icsd_649860	Pt ₃ Y ₇	36.175
icsd_067370	Co ₂ KSe ₂	71.536	icsd_104487	IrLi	187.213
icsd_069849	FeO ₄ Sr ₂	71.536	icsd_169398	CLa	187.213
icsd_106932	MnN	69.524	icsd_182014	NTc	187.213
icsd_167013	As ₂ F ₂ OSr ₂ Ti ₂	71.536	icsd_185568	NZr	187.213
icsd_168287	Hf ₂ Tl	71.536	icsd_185572	NRu	38.189
icsd_186572	Fe ₂ KS ₂	69.524	icsd_290430	N ₂ Ta	187.213
icsd_186573	Fe ₂ KSe ₂	71.536	icsd_290439	N ₂ Os	187.213
icsd_186574	Fe ₂ KTe ₂	71.536	icsd_073339	I ₃ LiSc	188.219
icsd_245748	Cl ₆ NbRb ₂	69.524	icsd_027140	Al ₈ FeMg ₃ Si ₆	189.225
icsd_246483	CoO ₄ Sr ₂	71.536	icsd_096905	Al ₉ FeMg ₃ Si ₅	189.225
icsd_420975	BaCo ₂ Ge ₂	139.537	icsd_030331	B ₂ V	65.486
icsd_425467	CaFe ₂ Si ₂	71.536	icsd_030416	B ₂ Cr	65.486
icsd_610297	As ₂ CsRu ₂	139.537	icsd_043664	B ₂ Mn	191.24

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

ICSD	Formula	MSG	ICSD	Formula	MSG
icsd_044581	B ₂ Ru ₃ Y	65.486	icsd_169410	ScSn	119.319
icsd_103634	FeSn	191.24	icsd_169766	CrTe	44.231
icsd_181506	S ₂ Ti	191.24	icsd_183160	CY	160.67
icsd_182350	CN ₃ Ta ₂	65.486	icsd_183166	CMo	119.319
icsd_182352	N ₃ OTa ₂	65.486	icsd_183198	CdN	44.231
icsd_240144	Mn ₆ Sn ₆ Y	65.486	icsd_184925	AsMn	44.231
icsd_260251	Co ₂ In ₉ K	191.24	icsd_191171	MnSn	119.319
icsd_415256	Co ₆ Ge ₆ Mg	191.241	icsd_191788	MnP	119.319
icsd_613892	B ₂ Fe	191.24	icsd_025596	F ₃ Nb	123.345
icsd_109145	I ₃ Nb	193.26	icsd_029096	BaFeO ₃	123.345
icsd_009497	AsMn	63.463	icsd_042929	InNTi ₃	65.486
icsd_010486	BaSe ₃ V	194.27	icsd_042930	CTi ₃ Tl	65.486
icsd_015520	BaO ₃ Rh	194.27	icsd_042931	NTi ₃ Tl	123.345
icsd_015908	InSc ₃	194.27	icsd_043417	OsSi	166.101
icsd_018130	Se ₂ Ta	63.463	icsd_043799	BaMoO ₃	123.345
icsd_020009	PoTi	194.27	icsd_043847	CaCo ₃	123.345
icsd_023405	Fe ₃ Ge	194.27	icsd_044385	RhSi	123.345
icsd_024569	Fe ₃ Sn	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 ₂ La	194.266	icsd_053125	Cr ₃ GaN	166.97
icsd_052503	TeTi	194.27	icsd_053461	Fe ₃ Ge	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 ₃ Sn	63.464	icsd_058107	AlOs	65.486
icsd_105427	NiTi	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 ₃ RbTi	63.457	icsd_076062	Mn ₃ NSn	166.101
icsd_191081	HCr	63.457	icsd_076790	CCO ₃ Mg	123.345
icsd_191785	MnP	63.464	icsd_077142	CoO ₃ Sr	65.486
icsd_603210	AlLa ₃	63.463	icsd_077152	CMgNi ₃	123.345
icsd_603351	GaMn ₃	63.463	icsd_088982	O ₃ SrV	123.345
icsd_625031	Co ₃ Si	63.464	icsd_091062	FeO ₃ Sr	123.345
icsd_631740	Fe ₃ Ga	63.463	icsd_099085	DSnTi ₃	123.345
icsd_640342	InRu ₃	63.463	icsd_103451	Fe ₃ Ga	65.486
icsd_640656	InTi ₃	194.266	icsd_103638	Fe ₃ Sn	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 ₄ Fe	63.464	icsd_104658	LaMg	123.345
icsd_052963	CoGe	146.1	icsd_104722	La ₃ Sn	123.345
icsd_187195	GeMn	146.1	icsd_104730	LaTi	123.345
icsd_616878	BiNiSe	19.27	icsd_104732	La ₃ Tl	166.101
icsd_652380	SiTe	146.1	icsd_106087	SnTi ₃	123.345
icsd_063230	BaS ₃ V	20.34	icsd_108129	CCO ₃ Sn	123.345
icsd_028647	CdKN ₃ O ₆	47.252	icsd_108903	CrO ₃ Sr	123.345
icsd_028648	CdN ₃ O ₆ Rb	47.252	icsd_155928	CoSi	123.345
icsd_028649	CdCsN ₃ O ₆	47.252	icsd_159440	MoN	123.345
icsd_028650	CdN ₃ O ₆ Tl	47.252	icsd_167812	Al ₃ V	123.345
icsd_042539	CoSe ₂	61.436	icsd_167814	Al ₃ Ti	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 ₂ Rh	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 ₂ V ₃	155.45	icsd_187483	O ₃ RhSr	123.345
icsd_181035	Cr _{0.25} Ga _{0.75} P	111.255	icsd_187637	O ₃ PbV	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 ₃ Sr	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 ₃ V	123.345

TABLE S66. 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 ₂ Lu ₂	12.58
icsd_236831	CoN	123.345	icsd_623661	Co ₂ Ge ₄ Y ₃	12.58
icsd_247066	Co ₃ InN	65.486	icsd_645402	Nb ₂ Se ₄ V	12.58
icsd_247648	AsLu	123.345	icsd_150696	Ca ₂ FeO ₆ Re	14.75
icsd_608581	AlMo	123.345	icsd_150258	LaMnO ₃	15.85
icsd_022412	SiV ₃	167.106	icsd_164176	BaFe ₂ O ₅ Y	47.252
icsd_102767	Cr ₃ Ga	167.105	icsd_670101	AgCuO ₂	47.252
icsd_106108	SnZr ₃	131.441	icsd_071520	FeNbTe ₂	53.328
icsd_187147	H ₃ Fe	66.496	icsd_083907	CrLaSb ₃	57.383
icsd_638098	Ge ₃ V	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_026881	OV	139.537	icsd_083987	LuMnSi	62.444
icsd_061323	CuO	71.536	icsd_191794	NiO ₃ Y	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	Clr	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 ₂ Ta	62.448
icsd_629532	D ₂ V	71.536	icsd_670835	CFeTa ₂	62.449
icsd_670177	FeSi ₂	139.537	icsd_670839	CFe ₂ W	62.448
icsd_027836	O ₄ Pt ₃	166.101	icsd_670840	CFeW ₂	62.449
icsd_041401	FeS ₂	29.102	icsd_057645	Al ₂ CoY	63.463
icsd_186518	FeO ₄ Si	31.125	icsd_195898	AsFe ₂ LaN	63.465
icsd_015003	FeSb ₂	34.156	icsd_200548	D ₃ CoZr	63.463
icsd_042726	FeS ₂	34.159	icsd_632057	FeGe ₂ Lu	63.462
icsd_042727	FeTe ₂	34.159	icsd_632162	FeGe ₂ Y	63.462
icsd_042728	CoTe ₂	34.159	icsd_072872	CoO ₄ Re	65.486
icsd_025678	CoTe ₂	58.397	icsd_016776	B ₂ CoW ₂	71.536
icsd_025679	FeTe ₂	58.397	icsd_040950	C ₄ CoSc ₃	71.536
icsd_026756	FeS ₂	58.397	icsd_072863	C ₄ FeSc ₃	71.536
icsd_041724	As ₂ Fe	58.393	icsd_167658	H ₂ PdTi ₂	71.536
icsd_041727	FeSb ₂	58.393	icsd_614261	B ₂ FeW ₂	71.536
icsd_042540	CoSe ₂	58.397	icsd_614775	B ₄ Mn ₂ Ta	71.536
icsd_076120	CoSb ₂	58.398	icsd_614782	B ₄ Mn ₂ W	71.536
icsd_194807	B ₄ Mn	58.393	icsd_416515	FePd ₂ Se ₂	72.544
icsd_610034	As ₂ Co	58.398	icsd_173487	NiO ₆ ReSr ₂	87.75
icsd_053146	CrN	59.407	icsd_042373	CoGe ₃ La	107.231
icsd_095957	Cu ₂ O ₃ Sr	59.409	icsd_059908	FeGe ₃ La	107.231
icsd_261526	ClLiNTi	59.41	icsd_181054	Cd _{0.5} Cr _{0.5} Te	25.59
icsd_152811	Fe ₂ N	60.417	icsd_047123	LaNiO ₂	123.345
icsd_185887	CrO ₂	60.424	icsd_051262	Ca ₂ ClCuNb ₃ O ₁₀	47.252
icsd_009496	AsMn	62.448	icsd_074163	Ba ₂ Cu ₂ O ₇ TIY	65.486
icsd_030412	MnP	62.445	icsd_150261	CoIn ₅ La	47.252
icsd_030449	BFe	62.447	icsd_150703	BaLaMn ₂ O ₆	47.252
icsd_043249	CoP	62.448	icsd_160691	CCr ₂ LaSi 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 ₄ Hf	65.486
icsd_093507	NiO ₃ Tl	62.446	icsd_623111	CoGa ₈ Lu ₂	65.486
icsd_670820	CaAl ₂ Fe	62.447	icsd_623236	CoGa ₅ Y	123.345
icsd_670821	CaIFe ₂	62.449	icsd_623237	CoGa ₈ Y ₂	123.345
icsd_164774	CaO ₃ Rh	63.464	icsd_623947	CoIn ₅ Y	47.252
icsd_187136	AsFeNa	63.462	icsd_623948	CoIn ₈ Y ₂	47.252
icsd_015927	MgO ₃ V	65.485	icsd_009967	CoNb ₄ P	124.353
icsd_020083	AlB ₂ Cr ₂	65.486	icsd_043233	CoNb ₄ Si	124.353
icsd_020322	AlB ₂ Fe ₂	65.485	icsd_053511	FeNb ₄ Si	66.496
icsd_025518	AlB ₂ Mn ₂	65.486	icsd_086378	FePTa ₄	124.353
icsd_645398	Nb ₂ Se ₄ V	8.32	icsd_623784	CoHf ₄ P	124.357
icsd_002371	CoSi ₂ Zr ₂	12.58	icsd_624637	CoPTa ₄	124.353
icsd_041746	CoSc ₂ Si ₂	12.58	icsd_624677	CoPZr ₄	124.353

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

ICSD	Formula	MSG	ICSD	Formula	MSG
icsd_632255	FeHf ₄ P	66.496	icsd_636559	GeHfMn	38.189
icsd_632795	FeNb ₄ P	66.496	icsd_637098	GeMnTa	189.225
icsd_043016	B ₂ FeW ₂	127.387	icsd_015995	Mn ₂ O ₃ Ta	65.486
icsd_613529	B ₂ CrNb ₂	65.486	icsd_044171	B ₂ Co ₃ Lu	65.486
icsd_613557	B ₂ CrTa ₂	65.486	icsd_044179	B ₂ Co ₃ Sc	191.238
icsd_080007	GeLaMn	59.407	icsd_044439	B ₂ LuRu ₃	65.486
icsd_080203	CoLaOP	67.506	icsd_054273	Mn ₆ ScSn ₆	65.486
icsd_085904	GeTiY	59.41	icsd_054928	Mn ₆ Sn ₆ Zr	65.486
icsd_088113	SiTiY	67.506	icsd_054930	HfMn ₆ Sn ₆	65.486
icsd_088208	LuSiTi	59.41	icsd_057416	LuMn ₆ Sn ₆	65.486
icsd_107617	GeLaTi	129.417	icsd_089433	Ge ₆ Mn ₆ Zr	65.486
icsd_162724	FeLaOP	59.407	icsd_186421	N ₃ Ta ₂ Ti	65.486
icsd_163496	AsFeLaO	59.407	icsd_104003	Ga ₃ Ti ₂ Zr ₃	63.464
icsd_168586	Fe ₂ O ₆ P ₂ Sc ₂ Sr ₄	59.407	icsd_168592	La ₆ Mn ₂ S ₁₀	193.26
icsd_180528	As ₂ Fe ₂ O ₆ Sc ₂ Sr ₄	59.407	icsd_604200	NiPb ₃ Zr ₅	63.463
icsd_420654	AsBa ₂ FeO ₃ Sc	59.407	icsd_624928	CoSb ₃ Zr ₅	63.464
icsd_617820	C ₂ FeSc	59.41	icsd_646460	NiSb ₃ Zr ₅	63.464
icsd_624599	CoPPd	67.506	icsd_659152	CrLa ₅ Pb ₃	193.26
icsd_636594	GeHfV	59.407	icsd_659153	La ₅ MnPb ₃	63.464
icsd_638931	HfSiV	59.407	icsd_659154	FeLa ₅ Pb ₃	193.26
icsd_061684	CCoY	47.252	icsd_659155	CoLa ₅ Pb ₃	63.464
icsd_061691	CCoLu	47.252	icsd_009966	Co ₃ Sc ₂ Si	194.27
icsd_068525	Fe ₄ P ₂ Sc	58.398	icsd_053483	Fe ₃ GeZr ₂	63.463
icsd_087172	Fe ₄ Si ₂ Zr	58.398	icsd_053558	Fe ₃ SiZr ₂	63.464
icsd_130032	Cu ₂ Hf ₂ In	136.501	icsd_057617	Al ₃ CoLu ₂	194.27
icsd_130034	Cu ₂ InZr ₂	136.501	icsd_076678	NiPZr	63.463
icsd_189495	Ni ₄ P ₂ Y	136.501	icsd_103807	GaMnPt	194.27
icsd_611100	As ₂ Ni ₄ Y	65.486	icsd_409622	Fe ₂ ILa ₂	63.464
icsd_633122	Fe ₄ P ₂ Zr	58.398	icsd_625123	Co _{1.5} Si _{0.5} W	63.465
icsd_053715	Ge ₂ Mn ₂ Y	71.536	icsd_670980	Nb ₂ Ni ₃ Si	194.27
icsd_082937	Mn ₂ Si ₂ Y	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 ₂ Si ₂	69.524	icsd_186188	Cr _{0.25} SeZn _{0.75}	111.255
icsd_107040	Ge ₂ LuMn ₂	71.536	icsd_076099	MnPdSb	44.231
icsd_191366	FeHfO ₆ Sr ₂	69.524	icsd_090397	FeSbZn	44.231
icsd_604549	B ₂ Fe ₂ Lu	139.537	icsd_107122	NbRhSb	44.231
icsd_614264	B ₂ Fe ₂ Y	139.537	icsd_108294	CoHfSb	44.231
icsd_632475	Fe ₂ LuSi 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 ₂ Sn	44.231
icsd_073974	AgNiO ₂	12.58	icsd_643329	MnPd ₂ Sn	139.537
icsd_193884	CrO ₂ Pd	12.58	icsd_671365	BiFePt	44.231
icsd_187087	LaNiO ₃	15.85	icsd_671366	BiCoPt	44.231
icsd_053016	CoNb ₃ S ₆	182.183	icsd_671367	BiNiPt	160.67
icsd_104913	MnNb ₃ S ₆	182.183	icsd_028908	LaO ₃ Ti	123.345
icsd_632811	FeNb ₃ Se ₆	20.31	icsd_028921	CoLaO ₃	123.345
icsd_643023	MnNb ₃ Se ₆	20.34	icsd_029119	LaMnO ₃	65.486
icsd_645400	Nb ₃ Se ₆ V	20.34	icsd_033667	CdO ₃ Ti	123.345
icsd_651111	S ₆ Ta ₃ V	20.34	icsd_044430	BLaRh ₃	123.345
icsd_020298	BFeNb	38.191	icsd_044864	Fe ₃ NPt	123.345
icsd_020876	CoGa ₂ Zr ₆	189.225	icsd_053142	Cr ₃ NPt	166.101
icsd_024185	MnNbSi	38.191	icsd_053506	Fe ₃ NPd	123.345
icsd_041156	GeMnPd	189.225	icsd_058547	AuNV ₃	166.97
icsd_042911	GeMnNb	38.191	icsd_076058	Mn ₃ NPt	166.101
icsd_061415	Fe ₂ S ₆ Ta ₉	38.191	icsd_076763	CFe ₃ Zn	65.486
icsd_082530	FeTe ₂ Zr ₆	38.191	icsd_076793	CCo ₃ Sc	123.345
icsd_083932	As ₂ CoZr ₆	189.225	icsd_076797	CCo ₃ Zn	123.345
icsd_086364	FeGeSc	38.191	icsd_077154	CMn ₃ Zn	123.345
icsd_096249	FeLu ₆ Sb ₂	38.191	icsd_051988	InMnPd ₂	166.101
icsd_156949	FeSb ₂ Zr ₆	38.191	icsd_053705	GeMnPd ₂	139.537
icsd_402701	Al ₂ FeZr ₆	38.191	icsd_057611	AlCo ₂ Hf	139.537
icsd_409925	GePdTi	38.189	icsd_057620	AlCo ₂ Nb	139.537
icsd_600156	GeMnSc	38.191	icsd_057634	AlCo ₂ Ta	139.537
icsd_610906	AsMnPd	38.191	icsd_058510	Au ₂ InTi	166.101
icsd_614205	BFeTa	38.191	icsd_076100	MnPd ₂ Sb	166.101
icsd_623801	CoHfSn	38.191	icsd_102441	Co ₂ GaNb	139.537
icsd_624869	Co ₂ S ₆ Ta ₉	38.189	icsd_102451	Co ₂ GaTa	139.537
icsd_626517	CrPPd	189.225	icsd_102483	Co ₂ HfSn	139.537
icsd_631770	FeGa ₂ Hf ₆	38.191	icsd_102554	Co ₂ NbSn	71.536
icsd_631856	FeGa ₂ Zr ₆	38.191	icsd_102687	Co ₂ SnZr	139.537

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

ICSD	Formula	MSG	ICSD	Formula	MSG
icsd_104945	MnPd ₂ Sn	139.537	icsd_020297	C ₂ Cr ₂ V	63.465
icsd_104980	Mn ₂ SnW	166.101	icsd_042629	CCr ₃ Ge	63.464
icsd_107955	AsMnPd ₂	166.101	icsd_044188	B ₃ CoV	63.463
icsd_185119	AlTiZr ₂	139.537	icsd_057009	C ₂ Cr ₃	63.465
icsd_190994	CMnSc ₂	71.536	icsd_189761	SnTi ₃	63.459
icsd_190996	MnSc ₂ Si	139.537	icsd_291338	CCr ₃ P	63.459
icsd_190998	GeMnSc ₂	139.537	icsd_291339	Cr ₃ NP	63.464
icsd_191000	MnSc ₂ Sn	71.536	icsd_609880	CAsCr ₃	63.465
icsd_108896	CoO ₃ Sr	11.5	icsd_637012	GeMnNi	63.462
icsd_000453	Ni ₃ S ₂ Sn ₂	12.58	icsd_043843	Al ₂ B ₂ Ru ₃	65.486
icsd_026173	CoMo ₂ S ₄	12.58	icsd_033704	B ₄ Cr ₃	71.536
icsd_026976	Cr ₃ Se ₄	12.58	icsd_044293	B ₄ Fe ₂ Mo	71.536
icsd_151873	CrFe ₂ Se ₄	12.58	icsd_044446	B ₄ Mn ₃	71.536
icsd_601347	Se ₄ Ti ₃	12.58	icsd_613166	B ₂ CoMo ₂	71.536
icsd_624884	CoS ₄ V ₂	12.58	icsd_614748	B ₄ Mn ₂ Mo	71.536
icsd_626655	CrS ₄ V ₂	12.58	icsd_066404	BaCuFeLuO ₅	35.167
icsd_626873	Cr ₃ Te ₄	12.58	icsd_167196	FeSe _{0.875}	25.59
icsd_633517	Fe ₂ Se ₄ V	12.58	icsd_023779	CrNNb	99.167
icsd_653087	Te ₄ TiV ₂	12.58	icsd_025751	Cr ₃ GeN	18.19
icsd_041858	AsCoS	14.75	icsd_093241	CuSb ₃ Ti ₂	115.285
icsd_602022	HFeTi	17.1	icsd_053505	FeNNi	65.486
icsd_081204	Ca ₂ FeO ₆ W	25.59	icsd_067711	Ba ₂ Fe ₃ O ₈ Y	47.252
icsd_629491	D ₂ FeTi	26.69	icsd_075730	Ba ₂ Ca ₂ Cu ₃ HgO ₈	123.345
icsd_632217	H ₂ FeTi	26.69	icsd_076202	MnRh ₂ Sb	47.252
icsd_020082	AlB ₄ Cr ₃	47.252	icsd_107862	AlNi ₃	65.486
icsd_190616	Co ₂ NbSn	51.295	icsd_157788	Co ₂ GaNi	65.486
icsd_194435	BNbRu	51.294	icsd_168837	H ₂ Mg _{0.5} Ti _{0.5}	127.397
icsd_263013	Fe ₃ O ₄	51.295	icsd_186722	Fe ₂ GaMn	123.345
icsd_421074	Ca ₂ Ge ₂ Ni ₃	51.295	icsd_187493	GaMnNi ₂	65.486
icsd_429116	BRuTa	51.295	icsd_187494	FeGaNi ₂	65.486
icsd_623100	Co ₂ GaLa	51.296	icsd_005431	B ₂ FeMo ₂	127.387
icsd_670573	CFe ₂	57.385	icsd_088317	B ₂ V ₃	65.486
icsd_612536	B ₂ BaNi ₂	58.398	icsd_613327	B ₂ Co ₅ Ta ₃	65.486
icsd_080372	C ₂ CrSc	59.407	icsd_644412	Mo ₃ Si ₂	65.486
icsd_646747	Ni ₃ Sn	59.411	icsd_016844	AsFe ₂	59.41
icsd_002421	CoMoP	62.446	icsd_042325	Mn ₂ Sb	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 ₂ P	62.447	icsd_165984	AsFeO ₃ Sr ₂ V	59.41
icsd_041149	MnRhSi	62.446	icsd_180529	As ₂ Cr ₂ Fe ₂ O ₆ Sr ₄	59.407
icsd_043521	CCo ₃	62.444	icsd_248374	CoMnSb	67.506
icsd_043686	PRu ₂	62.447	icsd_420653	AsCrFeO ₃ Sr ₂	59.407
icsd_044858	Co ₂ Si	62.449	icsd_200014	MoO ₆ Rh ₂	136.501
icsd_053079	CoSiTi	62.445	icsd_094079	FeMoO ₆ Sr ₂	139.537
icsd_055622	Mn ₃ Sn ₂	62.441	icsd_153292	GaMnNi ₂	139.537
icsd_076084	MnNiSi	62.448	icsd_246541	Ba ₂ FeMoO ₆	139.537
icsd_077856	PV ₂	62.445	icsd_617225	BiTi ₂	71.536
icsd_105931	Rh ₂ Sn	62.447	icsd_025760	AsCr ₃ N	140.543
icsd_165247	CoSiV	62.449	icsd_025775	CGeMn ₃	72.544
icsd_165250	CoFeSi	62.449	icsd_029132	F ₃ Fe	5.13
icsd_165256	CoNiSi	62.448	icsd_643223	Mn ₂ P	5.13
icsd_167128	CCoFe ₂	62.447	icsd_151457	AlO ₄ V 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 ₄ Fe	187.213
icsd_260757	BF ₃	62.446	icsd_042402	Fe ₂ P	38.191
icsd_603579	BCo ₂ Fe	62.447	icsd_043394	Mn ₂ P	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 ₂ Ge	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 ₂ Ti ₆	38.189
icsd_633291	Fe ₃ S	62.448	icsd_102686	CoSnZr	38.191
icsd_670816	CTi ₃	62.444	icsd_107550	Co ₂ P	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 ₃ Si	62.446	icsd_610094	AsCoNi	38.189

TABLE S69. 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 ₄ N	123.345
icsd_610532	AsFeV	38.191	icsd_044659	IrMn ₃ N	65.486
icsd_610883	AsMnNi	38.191	icsd_044865	Fe ₃ NNi	166.101
icsd_610927	AsMnTi	189.225	icsd_053132	Cr ₃ IrN	166.101
icsd_623254	CoGaZr	38.191	icsd_053143	Cr ₃ NRh	166.101
icsd_643230	MnPRh	189.225	icsd_053502	Fe ₄ N	123.345
icsd_643671	MnSiTi	189.225	icsd_077369	Fe ₁₁ Si ₅	123.345
icsd_036504	BCaNi ₄	191.24	icsd_077394	CRu ₃ V	123.345
icsd_102458	Co ₃ Ga ₂ Y	65.486	icsd_153274	Fe ₃ NRh	166.101
icsd_160914	H ₁₂ Fe ₅ La	65.486	icsd_183372	CuNNi ₃	65.486
icsd_601122	BFe ₄ Lu	65.486	icsd_052954	CoFe ₂ Ge	166.101
icsd_613036	BCo ₃ FeY	191.24	icsd_052958	Co ₂ FeSi	139.537
icsd_613133	BCo ₄ La	65.486	icsd_053002	Co ₂ MnSb	139.537
icsd_024359	Mn ₅ Si ₃	63.463	icsd_053007	Co ₂ MnSi	139.537
icsd_042585	Fe ₅ Si ₃	193.26	icsd_053080	Co ₂ SiTi	139.537
icsd_044386	Si ₃ Ti ₅	193.26	icsd_053462	Fe ₃ Ge	71.536
icsd_103996	Ga ₃ Ti ₅	193.26	icsd_053525	FeRu ₂ Si	166.101
icsd_103997	Ga ₄ Ti ₅	193.26	icsd_053545	Fe ₃ Si	139.537
icsd_191489	BSi ₃ V ₅	193.257	icsd_057600	AlCo ₂ Cr	139.537
icsd_609885	CAs ₃ V ₅	63.464	icsd_057607	AlCo ₂ Fe	139.537
icsd_613552	BCr ₅ Si ₃	63.464	icsd_057618	AlCo ₂ Mn	166.101
icsd_614407	BGe ₃ V ₅	63.464	icsd_057654	AlCrFe ₂	139.537
icsd_617535	CCr ₅ Si ₃	193.26	icsd_057662	AlCrNi ₂	139.537
icsd_637143	Ge ₃ Mo ₅	193.26	icsd_057695	AlCu ₂ Mn	166.101
icsd_638048	Ge ₃ Ti ₅	193.26	icsd_057793	AlFe ₃	166.101
icsd_643689	Mn ₃ Si ₃ V ₂	193.26	icsd_057806	AlFe ₂ Mn	71.536
icsd_644410	Mo ₅ Si ₃	193.26	icsd_057827	AlFe ₂ Ti	166.101
icsd_041921	GeMnNi	194.27	icsd_057832	AlFe ₂ V	166.101
icsd_052020	GeMn ₂	63.464	icsd_057986	AlMnRh ₂	166.101
icsd_053006	CoMnSi	63.464	icsd_076700	Ni ₂ SbTi	139.537
icsd_053460	Fe ₂ Ge	191.24	icsd_102318	Co ₂ CrGa	139.537
icsd_102582	CoNiSn	194.27	icsd_102385	CoFe ₂ Ga	166.101
icsd_102673	Co ₂ Sn	194.27	icsd_102386	Co ₂ FeGa	139.537
icsd_104976	Mn ₂ Sn	63.463	icsd_102392	Co ₂ FeIn	139.537
icsd_108289	Co ₂ Ge	63.463	icsd_102438	Co ₂ GaMn	166.101
icsd_108590	MnNiSi	63.463	icsd_102453	Co ₂ GaTi	139.537
icsd_163332	Mn ₂ Sb	194.27	icsd_102456	Co ₂ GaV	166.101
icsd_181132	FeSbV	63.463	icsd_102682	Co ₂ SnTi	139.537
icsd_182095	B ₄ Mo	63.463	icsd_102684	Co ₂ SnV	166.101
icsd_623495	CoGeMn	63.464	icsd_102755	CrFe ₂ Ga	139.537
icsd_624067	Co ₂ Mg	63.464	icsd_102996	Cu ₂ InMn	166.101
icsd_044660	IrMnSb	160.67	icsd_103057	Cu ₂ MnSn	166.101
icsd_053071	CoSbV	160.67	icsd_103469	Fe ₂ GaTi	139.537
icsd_053537	FeSbTi	160.67	icsd_103473	Fe ₂ GaV	71.536
icsd_053539	FeSbV	119.319	icsd_103615	FeRu ₂ Sn	166.101
icsd_054255	MnNiSb	44.231	icsd_103641	Fe ₂ SnTi	166.101
icsd_104498	IrMnSn	160.67	icsd_103644	Fe ₂ SnV	166.101
icsd_106496	CoSnTi	44.231	icsd_105376	Ni ₂ SnV	139.537
icsd_107127	RuSbTi	119.319	icsd_105933	Rh ₂ SnV	166.101
icsd_108492	GaRhTi	160.67	icsd_108436	Fe ₃ Ga	139.537
icsd_161713	MnNiSi	44.231	icsd_151206	Cu ₂ FeSn	166.101
icsd_184948	Mn ₂ Sb	44.231	icsd_151207	CoCu ₂ Sn	71.536
icsd_185079	CoSnV	119.319	icsd_185966	AlCo ₂ Ti	139.537
icsd_185882	AlTi ₂ Zn	119.319	icsd_185999	CrFe ₂ Sn	71.536
icsd_189696	AlTi ₂	119.319	icsd_186056	Fe ₂ InTi	166.101
icsd_189699	GaTi ₂	119.319	icsd_186059	AsFe ₂ Ti	166.101
icsd_189705	SiTi ₂	44.231	icsd_186060	Fe ₂ SbTi	71.536
icsd_189708	GeTi ₂	160.67	icsd_186065	Fe ₂ GeMn	166.101
icsd_189711	SnTi ₂	44.231	icsd_186721	Fe ₂ GaMn	166.101
icsd_190990	CoMnTe	119.319	icsd_188332	GaMn ₃	166.101
icsd_191683	FeTeV	119.319	icsd_416260	Co ₂ CrIn	139.537
icsd_191685	CrFeTe	44.231	icsd_608800	AlNi ₃	166.101
icsd_623808	Co ₂ HfSn	139.537	icsd_623481	Co _{8.8} Ge ₄ Mn _{3.2}	139.537
icsd_625319	Co ₂ SnZr	139.537	icsd_671340	GeRu ₂ V	166.101
icsd_670704	MnSiVZr	44.231	icsd_671341	Ru ₂ SbV	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 S70. 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 ₆ SbSr ₂	107.231	icsd_182323	NaO ₂ V	12.58
icsd_001029	CoI ₄ Rb ₂	11.53	icsd_250692	C ₂ CoN ₂ S ₂	12.58
icsd_002232	CuI ₂ O ₆	11.5	icsd_251654	CrI ₃	12.62
icsd_036581	HCuO ₅ STl	11.5	icsd_260368	H ₄ O ₁₀ V ₄	12.58
icsd_036582	HCuO ₅ SeTl	11.5	icsd_262639	Cl ₃ Tc	12.6
icsd_166586	F ₅ KNOOs	11.53	icsd_403035	Cl ₄ CrLi ₂	12.62
icsd_166587	CsF ₅ NOOs	11.53	icsd_423461	Br ₄ W	12.6
icsd_170771	MnNaO ₄ Rb ₂	11.54	icsd_602341	NiPS ₃	12.61
icsd_187148	H ₄ Fe	11.53	icsd_611574	As ₂ V	12.6
icsd_246090	Ca ₂ MnO ₆ Sb	11.54	icsd_624616	Co ₂ P ₂ S ₆	12.6
icsd_411140	Cl ₇ CsTi ₂	11.52	icsd_626521	CrPSe ₃	12.58
icsd_422751	CuNa ₂ O ₂	11.53	icsd_646145	NiPSe ₃	12.6
icsd_631817	FeGa ₂ Se ₄	111.255	icsd_647926	P ₂ Pd ₂ S ₆	12.61
icsd_246244	CaFeO ₂	18.19	icsd_648076	P ₂ S ₆ V ₂	12.61
icsd_102500	CoIn ₃	34.158	icsd_657314	Ni ₂ P ₂ S ₆	12.61
icsd_631756	FeGa ₃	34.158	icsd_670347	CaMnO ₃	12.62
icsd_150822	FeS ₂ Tl	119.319	icsd_108934	CrK ₃ O ₄	42.221
icsd_633509	FeSe ₂ Tl	119.319	icsd_108935	K ₃ MnO ₄	42.221
icsd_004073	CrI ₂	12.58	icsd_172506	GeMnTe ₄ Tl ₂	121.331
icsd_009485	H ₄ CuF ₂ O ₂	12.62	icsd_172507	MnSnTe ₄ Tl ₂	121.331
icsd_015596	H ₄ Cl ₂ MnO ₂	12.58	icsd_608538	Al ₂ MnTe ₄	42.221
icsd_015597	H ₄ Cl ₂ FeO ₂	12.62	icsd_639984	In ₂ MnTe ₄	42.221
icsd_016225	NiO ₆ Sr ₂ Te	12.62	icsd_659100	Ga ₂ MnSe ₄	42.221
icsd_016252	Fe ₂ P ₂ S ₆	12.61	icsd_004199	CoKO ₂	24.55
icsd_016270	MnNaO ₂	12.62	icsd_021072	F ₄ FeRb	47.252
icsd_017013	CoO	12.58	icsd_027689	CuF ₃ K	65.486
icsd_021055	Ba ₂ CuF ₆	12.62	icsd_027690	CrF ₃ K	47.252
icsd_022079	Br ₂ Cu	12.62	icsd_043457	CuF ₃ Tl	65.486
icsd_022080	Cl ₃ Cr	12.62	icsd_069675	Cs ₂ F ₅ Mn	123.345
icsd_022082	H ₄ Cl ₂ CoO ₂	12.58	icsd_075868	CaCuO ₂	123.345
icsd_022084	H ₄ Br ₂ MnO ₂	12.58	icsd_082218	F ₅ MnRb ₂	123.345
icsd_022085	H ₄ Br ₂ CoO ₂	12.58	icsd_109293	CuF ₃ Rb	65.486
icsd_023903	Br ₂ Cr	12.62	icsd_412972	Na ₅ NiO ₂ S	123.345
icsd_026108	Cl ₃ Mo	12.61	icsd_412978	CoNa ₅ O ₂ S	47.252
icsd_026609	NaNiO ₂	12.58	icsd_021110	CuF ₃ K	55.358
icsd_026667	Cl ₂ Cu	12.62	icsd_085499	F ₄ FeRb	127.387
icsd_030011	FeS ₂ Tl	12.61	icsd_245749	Cl ₆ K ₂ Nb	58.398
icsd_031320	C ₂ N ₂ NiS ₂	12.62	icsd_010454	Bi ₂ CaMn	59.407
icsd_042077	P ₂ V	12.61	icsd_015770	CoKO ₂	129.417
icsd_043898	As ₂ Cr	12.6	icsd_026458	LiMnP	59.407
icsd_047223	IrK ₄ O ₄	12.62	icsd_026459	AsLiMn	59.407
icsd_049021	KLiMnO ₂	12.6	icsd_026460	MnNaP	59.407
icsd_060263	D ₄ Cl ₂ CoO 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 ₄ IrO ₄	12.62	icsd_041869	CsMnSb	59.407
icsd_072389	Ca ₂ FeN ₂	12.61	icsd_041882	KMnP	59.407
icsd_075454	As ₂ Ba ₂ Mn ₂ O	12.61	icsd_041883	AsKMn	59.407
icsd_076548	NaSe ₂ V	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	ClKMnO ₅ P	129.417
icsd_100354	FeSe ₂ Tl	12.6	icsd_050989	ClMoO ₅ PRb	129.417
icsd_160556	CoO ₂	12.62	icsd_052758	CaGeMn	59.407
icsd_169194	CoO ₆ Pb ₂ Te	12.62	icsd_053707	GeMnSr	59.407
icsd_174134	CuLi ₂ O ₂	12.62	icsd_059359	Li ₂ O ₅ SiV	129.417

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.060736	BiMnNa	129.416	icsd.000406	CaCo ₂ Ge ₂	71.535
icsd.066948	GeMgMn	59.407	icsd.000407	Co ₂ Ge ₂ Sr	71.535
icsd.066949	CaMnSi	59.407	icsd.001139	Cl ₄ MnRb ₂	71.536
icsd.066950	CaMnSn	59.407	icsd.010463	CaFe ₂ P ₂	69.523
icsd.066951	MnSnSr	59.407	icsd.010466	Co ₂ P ₂ Sr	69.523
icsd.082639	BaCoS ₂	67.503	icsd.010467	Fe ₂ P ₂ Sr	139.536
icsd.086777	GeLi ₂ O ₅ V	129.417	icsd.010468	BaFe ₂ P ₂	69.523
icsd.088460	FFeO ₃ Sr ₂	67.503	icsd.015372	CuF ₄ K ₂	69.524
icsd.089590	KMnSb	59.407	icsd.021069	K ₂ NiO ₂	71.536
icsd.089594	MnPRb	59.407	icsd.032019	BaMn ₂ Sb ₂	71.535
icsd.089596	AsMnRb	59.407	icsd.041571	Cl ₄ CrCs ₂	71.536
icsd.089598	CsMnP	59.407	icsd.041794	As ₂ BaMn ₂	71.535
icsd.090122	ClCoO ₃ Sr ₂	67.506	icsd.053059	CoO	71.536
icsd.093508	ClFeO ₃ Sr ₂	59.407	icsd.065259	Cs ₂ CuF ₆	69.524
icsd.093509	BrFeO ₃ Sr ₂	67.503	icsd.073209	Na ₂ NiO ₂ Rb	139.537
icsd.096557	Ca ₂ ClFeO ₃	59.407	icsd.074889	CoCsK ₂ O ₂	69.524
icsd.162899	CrSe	59.407	icsd.100025	Bi ₂ MnSr	71.535
icsd.162900	MnSe	59.407	icsd.163209	As ₂ Fe ₂ Sr	71.535
icsd.162903	NiSe	129.417	icsd.166016	As ₂ CaFe ₂	71.535
icsd.163143	AsFeNa	59.407	icsd.167014	F ₂ OSb ₂ Sr ₂ Ti ₂	71.536
icsd.189939	FMnPSr	59.407	icsd.183149	Ba ₂ F ₂ Mn ₂ OSe ₂	71.536
icsd.189940	AsFMnSr	59.407	icsd.236760	O ₄ Sr ₂ Tc	71.536
icsd.189941	FMnSbSr	59.407	icsd.249687	Ba ₂ F ₂ Fe ₂ OSe ₂	71.536
icsd.248364	BaFMnSb	59.407	icsd.249690	F ₂ Fe ₂ OSe ₂ Sr ₂	71.536
icsd.248365	AsBaFMn	59.407	icsd.252590	BaBi ₂ Mn ₂	71.535
icsd.290482	H ₂ Ti	129.419	icsd.405782	CoO ₆ Pb ₂ Te	71.536
icsd.426033	BaBiFMn	129.416	icsd.420974	CaCo ₂ Si ₂	71.535
icsd.601586	BiKMn	129.416	icsd.425470	Co ₂ Si ₂ Sr	71.535
icsd.616575	BiCsMn	129.416	icsd.609848	As ₂ BaCo ₂	71.535
icsd.616824	BiMnRb	129.416	icsd.609849	As ₂ BaCr ₂	71.535
icsd.642150	LiMnSb	59.407	icsd.609899	As ₂ CaCo ₂	71.535
icsd.010293	Cl ₄ Re	13.68	icsd.610122	As ₂ Co ₂ Sr	71.535
icsd.063686	ClF ₆ O ₂ Ru	13.68	icsd.610273	As ₂ Cr ₂ Sr	71.535
icsd.067168	Cl ₇ CsTi ₂	13.67	icsd.004411	Cl ₃ MoO	14.77
icsd.186505	AsCaFFe	13.67	icsd.006024	CuF ₂	14.75
icsd.186508	AsFFeSr	13.67	icsd.006044	F ₆ Li ₂ Rh	14.75
icsd.000393	MnO ₂	65.486	icsd.010350	CrF ₆ Li ₂	14.75
icsd.001504	O ₂ V	136.501	icsd.015590	Cl ₃ CuK	14.77
icsd.009165	F ₂ Mn	136.499	icsd.015889	O ₂ V	14.77
icsd.009166	F ₂ Fe	58.398	icsd.020453	AgF ₂	14.79
icsd.009167	CoF ₂	136.499	icsd.023722	MoO ₂	14.77
icsd.009168	F ₂ Ni	65.486	icsd.026073	F ₆ Na ₃ Ni	14.79
icsd.015071	O ₂ Ru	136.499	icsd.027070	CrF ₆ Na ₃	14.79
icsd.016763	F ₂ Pd	58.398	icsd.027347	F ₆ Na ₃ V	14.79
icsd.024794	Cr ₂ O ₆ Te	58.395	icsd.030410	CuO ₆ Sb ₂	14.79
icsd.024795	Fe ₂ O ₆ Te	136.503	icsd.031827	CrF ₂	14.75
icsd.032552	F ₂ V	58.398	icsd.034602	CuF ₄ Na ₂	14.75
icsd.040344	FeO ₆ Sb ₂	58.398	icsd.038384	HClCuO	14.77
icsd.072387	CoLiN ₂ Sr ₂	136.501	icsd.042614	CoSb ₂	14.75
icsd.074565	F ₆ Li ₂ Mo	58.398	icsd.054136	Br ₃ CrIn	14.78
icsd.076024	O ₂ Ta	136.501	icsd.061038	K ₂ Mn ₂ O ₃	14.78
icsd.078778	CrF ₄	136.502	icsd.062655	F ₄ LiMn	14.79
icsd.080802	NiO ₆ Sb ₂	136.501	icsd.065510	I ₆ K ₂ Tc	14.75
icsd.084789	CuO ₆ Sb ₂	58.398	icsd.065785	F ₄ V	14.79
icsd.095778	F ₆ Li ₂ Rh	58.398	icsd.066201	Cl ₄ CrNa ₂	14.79
icsd.099714	MoO ₂	136.499	icsd.066315	F ₆ MnNa ₃	14.79
icsd.103447	FeGa ₃	58.395	icsd.067250	CrF ₄ Na ₂	14.79
icsd.108964	CoO ₆ Sb ₂	65.486	icsd.069801	MnO ₆ Se ₂	14.75
icsd.165210	F ₆ Li ₂ Ru	136.499	icsd.071455	F ₄ MnNa	14.79
icsd.168834	H ₂ Ti	58.398	icsd.074940	CoK ₂ O ₂	14.77
icsd.201756	F ₆ Na ₂ Nb	65.486	icsd.079451	CaIrO ₆ Sr ₂	14.75
icsd.262579	K ₃ NiO ₂	58.398	icsd.083473	Ca ₂ FeO ₆ Sb	14.75
icsd.290252	F ₆ Li ₂ V	136.501	icsd.084791	Ca ₃ O ₆ Re	14.79
icsd.412062	Co ₄ In ₁₂	58.398	icsd.084949	HMnO ₂	14.77
icsd.418676	CrF ₆ Li ₂	58.398	icsd.098698	HCuFO	14.75
icsd.424578	Cs ₃ NiO ₂	58.398	icsd.153001	Ca ₂ CoO ₆ Te	14.75
icsd.424579	NiO ₂ Rb ₃	58.398	icsd.153002	CoO ₆ Sr ₂ Te	14.79
icsd.074985	B ₄ Mn ₄	67.503	icsd.165398	F ₄ Ru	14.75
icsd.000404	BaGe ₂ Mn ₂	71.535	icsd.169193	CoO ₆ Pb ₂ Te	14.75
icsd.000405	BaMn ₂ Sn ₂	139.536	icsd.173152	O ₂ Tc	14.77

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.182568	CaO ₆ ReSr ₂	14.75	icsd.042163	F ₆ HgRh	2.4
icsd.185809	AsFeS	14.77	icsd.054140	MnPSe ₃	2.6
icsd.190486	Ca ₂ InO ₆ Os	14.75	icsd.054141	FePSe ₃	2.6
icsd.190774	C ₂ NiO ₄	14.75	icsd.056890	Fe ₂ P ₂ Se ₆	2.6
icsd.193723	MnS ₂	14.75	icsd.059175	KO ₈ S ₂ V	2.4
icsd.202451	CuO ₃ Te	14.77	icsd.059343	BaCo ₂ O ₈ P ₂	148.19
icsd.202918	CoF ₄ Li	14.75	icsd.061217	IrLi ₈ O ₆	2.4
icsd.238316	InO ₆ OsSr ₂	14.79	icsd.063304	FeI ₁₂ Y ₇	2.4
icsd.239557	Cl ₃ CuTi	14.77	icsd.063353	AsNaNiO ₄	2.6
icsd.250364	Cl ₄ V	14.75	icsd.063544	AsKNiO ₄	2.6
icsd.290251	F ₆ Li ₂ V	14.75	icsd.069591	GeMnO ₃	2.6
icsd.290789	CrO ₆ SbSr ₂	14.75	icsd.071020	Cr ₂ Si ₂ Te ₆	148.17
icsd.290790	Ca ₂ CrO ₆ Sb	14.79	icsd.076421	Br ₃ Fe	2.4
icsd.411050	Cl ₆ Na ₃ Ti	14.75	icsd.079165	B ₂ MnO ₆ Sn	148.17
icsd.421461	AgF ₄ K ₂	14.79	icsd.079268	Cr ₂ Ge ₂ Te ₆	148.17
icsd.425100	B ₄ Mn	14.75	icsd.095776	F ₆ LiRh	148.17
icsd.425149	AgF ₄ Na ₂	14.75	icsd.095777	F ₆ IrLi	148.17
icsd.610526	AsFeSe	14.77	icsd.165203	F ₆ LiRu	2.4
icsd.610529	AsFeTe	14.78	icsd.165206	F ₆ LiOs	148.17
icsd.633086	FePS	14.77	icsd.165208	F ₆ LiPt	2.4
icsd.633093	FePSe	14.77	icsd.165215	F ₆ KRh	2.4
icsd.633399	FeSbSe	14.77	icsd.169192	CoO ₆ Pb ₂ Te	148.17
icsd.633405	FeSbTe	14.77	icsd.174290	Ba ₂ BiIrO ₆	2.4
icsd.008000	CuF ₃ K	140.545	icsd.182435	Mn ₃ O ₆ Te	2.6
icsd.042520	Sb ₂ Ti	140.543	icsd.240981	BaF ₆ Ir	148.17
icsd.052331	Sb ₂ V	72.541	icsd.251655	CrI ₃	148.17
icsd.069656	CuF ₃ Rb	69.524	icsd.260062	As ₂ BaCo ₂ O ₈	148.17
icsd.075412	F ₃ KMn	72.544	icsd.280167	BaNi ₂ O ₈ P ₂	2.6
icsd.076127	BCr ₂	72.541	icsd.408324	Ca ₂ Li ₆ Mn ₂ N ₆	148.19
icsd.086811	CrSb ₂	140.543	icsd.412874	Li ₆ Mn ₂ N ₆ Sr ₂	148.19
icsd.169765	CrF ₃ K	72.544	icsd.418671	CrF ₆ Na	148.17
icsd.174206	MoO ₃ Sr	72.544	icsd.418672	CrF ₆ K	2.4
icsd.183452	O ₃ SrTc	140.541	icsd.418673	CrF ₆ Rb	2.4
icsd.248378	BaIrO ₃	140.541	icsd.419467	Ba ₆ N ₆ OOs ₂	2.4
icsd.031149	Fe ₂ Li ₂ O ₄	70.53	icsd.424895	BaFe ₂ O ₈ P ₂	2.6
icsd.043437	FeLiO ₂	141.556	icsd.626809	CrSiTe ₃	148.17
icsd.164158	LiO ₂ Ti	141.556	icsd.643237	Mn ₂ P ₂ Se ₆	2.6
icsd.091527	KNiO ₉ P ₃	146.1	icsd.670349	CaMnO ₃	148.17
icsd.162264	BiFeO ₃	1.1	icsd.060313	IKNiO ₆	5.13
icsd.193740	H ₄ As ₃ MnNS ₆	1.1	icsd.201056	C ₆ Au ₃ CoKN ₆	5.13
icsd.073736	CsO ₈ S ₂ V	2.4	icsd.249724	C ₆ Au ₃ KN ₆ Ni	5.13
icsd.245667	CsFeO ₈ S ₂	2.4	icsd.002790	CrP ₄	15.87
icsd.250709	BaCo ₂ O ₈ P ₂	147.15	icsd.006286	O ₃ V ₂	15.88
icsd.002552	Cl ₃ MnNa	148.17	icsd.015557	FeKS ₂	15.88
icsd.010343	CaCrF ₆	2.4	icsd.038315	P ₄ V	15.87
icsd.010344	CrF ₆ Mg	2.4	icsd.040780	FeKSe ₂	15.88
icsd.010347	CrF ₆ Hg	148.17	icsd.040781	FeRbSe ₂	15.87
icsd.015108	F ₆ NiPb	2.4	icsd.202381	FeRbS ₂	15.88
icsd.016316	Mo ₃ Se ₄	148.19	icsd.075550	FeO ₈ RbSe ₂	5.15
icsd.022081	Cl ₃ Cr	148.17	icsd.004266	FeO ₄ P	152.35
icsd.025010	F ₆ MnSn	2.4	icsd.025813	BaCoO ₂	5.13
icsd.025011	F ₆ FeSn	2.4	icsd.010424	Ni ₃ S ₂	5.15
icsd.025014	CoF ₆ Sn	148.17	icsd.110773	LiMnTe ₂	8.34
icsd.025015	F ₆ NiSn	148.17	icsd.182698	H ₄ Ni ₃ O ₉ Si ₂	157.55
icsd.025016	CuF ₆ Sn	148.17	icsd.022093	Cl ₃ Ru	9.39
icsd.027014	As ₂ BaNi ₂ O ₈	2.6	icsd.001372	HCrO ₂	160.67
icsd.027500	Cl ₃ Fe	148.19	icsd.001373	DCrO ₂	160.67
icsd.027664	F ₆ KOs	148.17	icsd.024315	Se ₂ Ta	8.34
icsd.029203	MnO ₃ Sn	2.6	icsd.029312	NiS	160.65
icsd.033288	Cl ₂ CoO ₈	148.17	icsd.036207	Fe ₃ O ₇ P	160.67
icsd.033289	Cl ₂ NiO ₈	2.4	icsd.042596	NiSe	8.32
icsd.035145	I ₁₂ Zr ₆	2.4	icsd.043410	S ₂ Ta	8.32
icsd.038236	Cl ₃ Ti	2.6	icsd.069571	H ₆ F ₃ O ₃ V	8.34
icsd.038237	Cl ₃ V	2.4	icsd.077990	RbS ₂ Ti	8.32
icsd.039242	Br ₃ Ti	2.4	icsd.088852	AuCrS ₂	8.34
icsd.041539	Cl ₁₂ Zr ₆	148.19	icsd.201396	CrS ₂ Tl	160.67
icsd.041540	Br ₁₂ Zr ₆	148.19	icsd.401027	Cl ₈ Na ₂ Ti ₃	8.32
icsd.042159	F ₆ MgRh	2.4	icsd.607619	Al ₂ FeS ₄	8.32
icsd.042160	CaF ₆ Rh	2.4	icsd.608507	Al ₂ MnS ₄	8.32
icsd.042161	F ₆ RhZn	2.4	icsd.626736	CrSe ₂ Tl	8.32

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_634670	Ga ₂ MnS ₄	8.34	icsd_246907	I ₂ V	12.58
icsd_639980	In ₂ MnSe ₄	160.67	icsd_416038	NaO ₈ Rb ₃ Ru ₂	12.6
icsd_641335	KS ₂ Ti	8.32	icsd_416040	K ₃ NaO ₈ Ru ₂	12.6
icsd_644994	NaS ₂ V	8.32	icsd_425912	Cs ₂ F ₆ Tc	164.89
icsd_015299	BiFeO ₃	9.39	icsd_425914	F ₆ K ₂ Tc	164.89
icsd_028917	BaFeO ₃	9.39	icsd_425915	F ₆ Na ₂ Tc	164.89
icsd_200999	Li ₂ O ₃ Re	9.37	icsd_425918	F ₆ Rb ₂ Tc	164.89
icsd_246425	BiCrO ₃	161.69	icsd_626052	CrGa ₂ S ₄	164.89
icsd_252433	LiO ₃ Os	161.69	icsd_631804	Fe ₂ Ga ₂ S ₅	12.6
icsd_001838	BaFe ₄ O ₈ Sr	12.58	icsd_632443	FeLi ₂ S ₂	12.62
icsd_009484	C ₆ D ₃ CoN ₆	162.77	icsd_634664	Ga ₂ Mn ₂ S ₅	164.88
icsd_015174	BaCaFe ₄ O ₈	12.58	icsd_000071	Fe ₃ Sn ₂	166.101
icsd_029035	Cl ₃ Ti	12.6	icsd_001846	Cl ₈ Mn ₃ Na ₂	166.101
icsd_080349	As ₂ NiO ₆	12.58	icsd_004059	Cl ₂ Fe	12.62
icsd_080350	As ₂ CoO ₆	162.77	icsd_006038	BaF ₆ Rh	166.101
icsd_187098	As ₂ O ₆ Pd	12.58	icsd_006152	CoNaO ₂	12.58
icsd_201755	F ₆ Li ₂ Nb	12.62	icsd_009457	Ba ₃ Cr ₂ O ₈	166.101
icsd_248351	O ₆ Ru ₂ Sr	162.75	icsd_010341	BaCrF ₆	166.101
icsd_291234	MnO ₆ Sb ₂	12.62	icsd_010342	CrF ₆ Sr	166.101
icsd_032730	CaCoF ₆ Li	15.87	icsd_014208	Cl ₂ Ni	12.58
icsd_032732	CaF ₆ LiNi	15.88	icsd_015558	CrNaS ₂	12.58
icsd_032733	F ₆ LiNiSr	15.88	icsd_015939	Cl ₂ Co	12.62
icsd_062035	Cl ₆ CrNa ₃	15.89	icsd_020372	BiFeO ₃	166.101
icsd_073132	AlF ₆ LiPd	15.89	icsd_022106	Br ₂ Ni	12.58
icsd_073985	CaCrF ₆ Li	163.83	icsd_022108	I ₂ Ni	166.101
icsd_078748	F ₆ GaLiPd	15.89	icsd_022285	HCoO ₂	12.58
icsd_183024	Cl ₆ MoNa ₃	15.87	icsd_024594	LiO ₂ V	12.58
icsd_015901	Cl ₂ V	12.62	icsd_024595	CrNaO ₂	166.101
icsd_016303	LiS ₂ V	12.62	icsd_025005	Ba ₂ NiO ₆ Te	166.1
icsd_022074	Cl ₉ Cs ₃ Fe ₂	164.88	icsd_025723	CrKS ₂	166.101
icsd_023591	H ₂ MnO ₂	164.89	icsd_026305	NaS ₂ Ti	12.62
icsd_026233	CrLiS ₂	12.62	icsd_028692	F ₆ KRu	12.58
icsd_028101	H ₂ NiO ₂	164.89	icsd_028693	F ₆ RbRu	12.58
icsd_028779	F ₆ K ₂ Rh	12.62	icsd_028694	CsF ₆ Ru	12.58
icsd_028780	F ₆ Rb ₂ Rh	12.62	icsd_028783	F ₃ Ti	166.101
icsd_033673	I ₂ Mn	164.89	icsd_029011	FeO ₂ Tl	166.1
icsd_037327	Li ₂ MnO ₂	164.89	icsd_029225	CoLiO ₂	12.58
icsd_039512	As ₂ Mn ₂ Zn	12.6	icsd_030114	F ₆ NiSr	166.101
icsd_041789	CaMn ₂ Sb ₂	12.6	icsd_031679	CrNaSe ₂	166.101
icsd_041790	Mn ₂ Sb ₂ Sr	12.61	icsd_032551	Fe ₂ Ga ₂ S ₅	12.61
icsd_041791	Bi ₂ CaMn ₂	12.6	icsd_033752	Cl ₂ Mn	166.101
icsd_041792	As ₂ CaMn ₂	164.89	icsd_035396	BaF ₆ Ni	12.62
icsd_041793	As ₂ Mn ₂ Sr	12.6	icsd_037157	FeNaO ₂	12.58
icsd_044908	LiTe ₂ Ti	12.58	icsd_040267	CrKO ₂	166.101
icsd_049017	CaMn ₂ P ₂	12.6	icsd_041814	Sb ₂ V ₃	12.58
icsd_049019	Mn ₂ P ₂ Sr	12.6	icsd_042158	F ₆ RhSr	166.101
icsd_052364	Br ₂ Co	12.58	icsd_043439	NaO ₂ Ti	12.58
icsd_052365	Br ₂ Fe	12.62	icsd_051207	FeLiO ₂	166.101
icsd_052368	CoI ₂	12.58	icsd_061276	F ₆ MnRb ₂	12.58
icsd_052369	FeI ₂	12.58	icsd_061692	IrKLi ₆ O ₆	166.101
icsd_059230	Ga ₂ NiS ₄	12.58	icsd_064764	DCO ₂	12.58
icsd_060250	Br ₂ Mn	164.89	icsd_067500	Br ₂ Mn	166.101
icsd_064831	Cl ₂ Fe	12.62	icsd_067701	Fe ₂ O ₄ Y	12.62
icsd_071421	Li ₂ NiO ₂	164.89	icsd_071536	CoK ₂ O ₆ Se ₂	12.58
icsd_071996	D ₈ FeMg ₂ Sr	164.89	icsd_071540	K ₂ MnO ₆ Se ₂	166.101
icsd_072831	F ₆ NbRb ₂	12.58	icsd_074030	Ba ₂ IrO ₆ Sr	166.101
icsd_072832	Cs ₂ F ₆ Nb	12.62	icsd_074680	Cl ₁₂ OsS ₂	12.58
icsd_079007	CrTe ₂ Tl	164.89	icsd_076541	NaS ₂ V	12.62
icsd_086519	S ₂ V	12.58	icsd_076959	NiO	12.58
icsd_086520	Se ₂ V	12.62	icsd_077597	NaSe ₂ V	12.62
icsd_088722	CoO ₂	12.58	icsd_085055	Cr ₂ O ₈ Sr ₃	166.1
icsd_088940	H ₂ CoO ₂	12.58	icsd_097758	CrLiO ₂	166.101
icsd_095779	F ₆ IrK ₂	12.62	icsd_108892	Ni ₃ Pb ₂ Se ₂	12.62
icsd_100706	FeGa ₂ S ₄	12.58	icsd_108893	Ni ₃ S ₂ Tl ₂	12.58
icsd_152482	Ba ₃ CaO ₉ Ru ₂	164.88	icsd_165117	K ₃ Mn ₂ O ₈	166.101
icsd_159909	Fe ₂ K ₃ NaO ₈	12.6	icsd_166489	KS ₂ Ti	12.58
icsd_182700	N ₃ V ₂	164.89	icsd_170135	CMnN ₂	166.101
icsd_240955	F ₆ IrRb ₂	12.62	icsd_170347	NaO ₂ Ru	12.62
icsd_240956	Cs ₂ F ₆ Ir	12.62	icsd_280045	Ba ₃ Mn ₂ O ₈	12.6
icsd_246906	Br ₂ V	12.58	icsd_291388	Cs ₂ Cu ₃ F ₁₂ Sn	12.62

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_401026	Cl ₈ Na ₂ Ti ₃	166.97	icsd_002782	Br ₃ CsMn	63.462
icsd_407802	Ba ₂ MnO ₆ Te	12.58	icsd_008193	BaS ₃ V	63.462
icsd_420137	NaO ₂ V	12.58	icsd_009704	Br ₃ MnRb	194.268
icsd_425834	H ₆ Cl ₂ Cu ₃ O ₆ Zn	12.62	icsd_010331	BaMnO ₃	63.462
icsd_640140	In ₂ Ni ₃ Se ₂	12.58	icsd_015011	Br ₃ NiRb	194.268
icsd_641350	KS ₂ Zr	12.58	icsd_015092	CsF ₃ Ni	63.463
icsd_670082	AuCrO ₂	12.58	icsd_016360	Ba ₂ Mn ₂ OSb ₂	194.271
icsd_670084	AuFeO ₂	166.101	icsd_016361	Ba ₂ Bi ₂ Mn ₂ O	194.271
icsd_001462	O ₃ Ti ₂	15.85	icsd_016773	AsTi	63.461
icsd_001473	O ₃ V ₂	15.88	icsd_023874	BaMnO ₃	63.463
icsd_005208	CCoO ₃	167.103	icsd_024305	Cl ₃ CoRb	63.463
icsd_015840	Fe ₂ O ₃	167.103	icsd_026453	CsI ₃ V	63.462
icsd_016649	F ₃ Ti	15.85	icsd_027511	Cl ₃ CoCs	63.464
icsd_016671	F ₃ Fe	15.89	icsd_029284	CPV ₂	63.461
icsd_016672	CoF ₃	167.103	icsd_029302	FeS	63.462
icsd_016673	F ₃ Ru	15.85	icsd_029305	CoS	63.462
icsd_025781	Cr ₂ O ₃	167.106	icsd_029308	FeSe	63.457
icsd_025828	CrF ₃	15.85	icsd_029310	NiSe	63.457
icsd_026629	F ₃ Mo	15.85	icsd_029313	NiS	194.268
icsd_028556	CMnO ₃	167.103	icsd_042444	PV	63.463
icsd_030624	F ₃ V	15.85	icsd_042541	CoSe	63.462
icsd_030662	Ba ₃ NiO 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 ₃ V	15.89	icsd_049747	Cl ₃ RbTi	63.462
icsd_061067	CNiO ₃	15.85	icsd_049748	Cl ₃ CsTi	63.462
icsd_100678	CFeO ₃	15.85	icsd_049912	Fe ₂ Ga ₂ S ₅	63.46
icsd_252432	LiO ₃ Os	167.103	icsd_052121	STi	194.268
icsd_402039	BO ₃ Ti	15.85	icsd_052509	TeV	63.462
icsd_094318	BLiMnO ₃	174.135	icsd_056288	HCoO ₂	63.457
icsd_036502	Ba ₃ FeN ₃	11.53	icsd_058188	AlTi ₃	63.461
icsd_072920	S ₄ V ₃	11.53	icsd_058714	Be ₂ Mn	63.461
icsd_095740	CBaF ₂ MnO ₃	176.145	icsd_058752	Be ₂ V	63.461
icsd_168997	FeO ₄ P	21.41	icsd_059371	Cl ₃ CsNi	194.268
icsd_002769	BaFe ₂ O ₄	20.34	icsd_071010	FeInO ₃	194.266
icsd_022092	Cl ₃ Ru	185.2	icsd_076218	MnSe	63.457
icsd_002064	Cl ₃ CsCu	36.174	icsd_076802	CCr ₂ Ge	63.461
icsd_002590	Br ₃ CrCs	186.205	icsd_084212	Cl ₃ CuRb	194.268
icsd_008105	CrCsI ₃	186.205	icsd_103991	GaTi ₃	63.461
icsd_010206	Cl ₃ CrCs	186.205	icsd_154258	CsI ₃ Ti	63.457
icsd_025578	F ₆ MnRb ₂	36.175	icsd_155189	Cl ₃ CoTi	63.462
icsd_042493	NiS	186.205	icsd_157935	MnO ₃ Sr	63.459
icsd_043458	CoO	36.172	icsd_169572	NiS ₂	63.465
icsd_044765	MnS	36.172	icsd_174041	Br ₃ CsFe	63.457
icsd_053528	FeS	36.176	icsd_181100	CPTa ₂	63.461
icsd_060417	F ₆ K ₂ Mn	186.207	icsd_183361	CCr ₂ Si	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 ₃ CsV	63.462
icsd_262928	MnO	36.172	icsd_201830	Cl ₃ RbV	63.462
icsd_281495	ClFeN ₃ O ₃	36.172	icsd_249387	CCoN ₂	63.457
icsd_643594	MnSe	36.172	icsd_249388	CN ₂ Ni	194.268
icsd_043671	CRu	38.191	icsd_290431	N ₂ Ta	63.461
icsd_088670	BaCoO ₃	38.191	icsd_300249	Cl ₃ CsFe	63.462
icsd_022091	Cl ₃ Ru	40.206	icsd_410394	Cs ₂ F ₆ Ni ₂	63.463
icsd_002278	CrCsF ₄	189.224	icsd_419223	CFeN ₂	63.462
icsd_096248	FeSb ₂ Y ₆	38.191	icsd_423829	Br ₃ CsNi	194.268
icsd_411152	Li ₅ N ₃ Ni ₃	38.189	icsd_423830	CsI ₃ Ni	63.457
icsd_187196	GeMn	19.27	icsd_425293	CrKO ₂	194.268
icsd_182351	N ₄ Ta ₂	65.486	icsd_624986	Co _{1.82} Se _{2.08}	63.462
icsd_004068	Br ₃ Zr	63.462	icsd_633476	Fe _{1.82} Se _{2.08}	63.457
icsd_022090	Cl ₃ Ru	193.259	icsd_636809	GeLaLi ₂	63.461
icsd_023163	Cl ₃ Zr	63.457	icsd_657109	Co _{1.82} S _{2.08}	63.462
icsd_023172	I ₃ Ti	63.462	icsd_659040	Fe _{2.85} N _{1.14}	63.462
icsd_023946	I ₃ Zr	63.462	icsd_670081	AuCoO ₂	63.462
icsd_023947	HfI ₃	193.259	icsd_670893	CMo	63.461
icsd_026069	Cl ₃ Ti	193.259	icsd_005250	FeSi	19.27
icsd_413691	Br ₃ Ru	63.462	icsd_016837	CrSi	19.25

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_016838	MnSi	146.1	icsd_041209	F ₂ Pd	205.33
icsd_016839	CoSi	19.27	icsd_066939	O ₂ Ru	61.436
icsd_020309	AsNiS	19.27	icsd_166458	N ₂ Os	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 ₂ Pd	198.9	icsd_169409	GeSc	160.67
icsd_624862	CoSSb	19.25	icsd_181079	CrN	160.67
icsd_002896	CuO ₆ S ₂ Tl ₂	2.4	icsd_181324	MnTe	44.231
icsd_006240	Ba ₂ CuO ₆ Te	2.6	icsd_183168	CTc	119.319
icsd_018115	As ₂ CuO ₈ Zn ₂	2.4	icsd_186876	MoP	160.67
icsd_023334	MnP ₄	2.6	icsd_192816	AsLiMn	44.231
icsd_036208	Fe ₂ O ₇ P ₂	2.6	icsd_236783	NV	160.67
icsd_036514	CuF ₆ Sn	2.4	icsd_236787	MnN	160.67
icsd_039784	Br ₃ Ti	2.6	icsd_671343	CrSe	160.67
icsd_050444	Cs ₄ CuO ₇ Si ₂	2.4	icsd_671386	SeV	44.231
icsd_051505	AgF ₆ Sn	2.4	icsd_671387	TeV	160.67
icsd_059585	FeNa ₄ O ₄	2.4	icsd_015246	CoF ₃ K	166.101
icsd_059721	AsBiMnO ₅	2.6	icsd_015423	F ₃ KMn	65.486
icsd_062544	AuCuF ₅	2.4	icsd_015424	F ₃ FeK	166.101
icsd_062676	CrNa ₄ O ₄	2.4	icsd_015426	F ₃ KNi	166.101
icsd_063058	As ₂ CuNa ₄ O ₈	2.4	icsd_023167	Cl ₃ MnTl	65.486
icsd_065186	AgF ₁₂ Sb ₂	2.4	icsd_028145	F ₃ KV	123.345
icsd_066023	Cl ₁₂ Te ₄ W ₂	2.4	icsd_028146	F ₃ RbV	123.345
icsd_069994	H ₂ O ₅ SeV	2.4	icsd_030612	F ₃ Mo	65.486
icsd_072461	H ₆ CuN ₄ O ₄	2.4	icsd_030613	F ₃ Ta	166.101
icsd_074682	Cl ₁₂ OsTe ₂	2.4	icsd_043722	F ₃ MnRb	123.345
icsd_078789	Cl ₆ ISe ₆ W	2.4	icsd_044616	RuSi	166.101
icsd_079879	AgBi ₂ F ₁₂	2.4	icsd_049583	CsF ₃ Fe	166.101
icsd_080430	KMnO ₈ Se ₂	2.4	icsd_049586	F ₃ FeRb	166.101
icsd_084620	Cl ₅ Mo	2.4	icsd_058151	AlRh	65.486
icsd_085404	CuK ₆ O ₈ Si ₂	2.4	icsd_060611	F ₃ NaV	166.101
icsd_085405	CuO ₇ Rb ₄ Si ₂	2.4	icsd_069360	O ₃ RuSr	166.101
icsd_087958	H ₄ FeK ₂ O ₁₀ S ₂	2.4	icsd_071994	MoO ₃ Sr	166.101
icsd_092916	AsBiNiO ₅	2.6	icsd_073166	F ₃ PdRb	65.486
icsd_096783	H ₄ K ₂ MnO ₁₀ Se ₂	2.4	icsd_073167	F ₃ KPd	65.486
icsd_098683	H ₄ CoNa ₂ O ₁₀ Se ₂	2.4	icsd_102423	CoGa	65.486
icsd_098684	H ₄ Na ₂ NiO ₁₀ Se ₂	2.4	icsd_103950	GaRu	65.486
icsd_098686	H ₄ CoK ₂ O ₁₀ Se ₂	2.4	icsd_109076	O ₃ SrTc	123.345
icsd_099580	Co ₂ Na ₆ O ₆	2.4	icsd_168836	H ₂ Mg _{0.25} Ti _{0.75}	166.97
icsd_156225	H ₄ Ca ₂ MnO ₁₀ P ₂	2.4	icsd_168900	BTc	65.486
icsd_166313	NaO ₆ Si ₂ Ti	2.6	icsd_168902	CaMnO ₃	123.345
icsd_171007	Ca ₂ Cl ₂ CuO ₁₀ Te ₄	2.4	icsd_236833	NNi	166.101
icsd_171656	F ₆ O ₂ Rh	2.4	icsd_237730	BaO ₃ Os	65.486
icsd_172335	C ₂ CuF ₆ O ₆ S ₂	2.4	icsd_671082	CaO ₃ Tc	123.345
icsd_173748	F ₂ O ₇ Te ₂ V ₂	2.6	icsd_671086	BaO ₃ Tc	123.345
icsd_174291	Ba ₂ BiIrO ₆	2.4	icsd_671397	F ₃ NiRb	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 ₂ O ₈ P ₂	2.6	icsd_106097	SnV ₃	167.105
icsd_240930	Cu ₂ Na ₂ O ₁₁ Si ₄	2.6	icsd_009864	MnO	139.537
icsd_409506	Cs ₆ NiO ₈ Si ₂	2.4	icsd_009865	CoO	166.101
icsd_411522	F ₁₂ MnSb ₂	2.4	icsd_009866	NiO	71.536
icsd_415445	O ₅ PSnV	2.4	icsd_018007	MnS	139.537
icsd_415768	Cl ₈ NW ₂	2.4	icsd_024251	MnSe	139.537
icsd_418858	Br ₂ CoO ₃ Sb ₂	2.6	icsd_027856	FeO	71.536
icsd_423336	Cs ₄ FeO ₃	2.6	icsd_037412	CrN	139.537
icsd_423462	Br ₅ W	2.4	icsd_040125	OTi	71.536
icsd_424465	Br ₁₀ CoY ₆	2.4	icsd_065410	F ₂ Ti	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 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_002258	DCrO ₂	31.125	icsd_016013	ClFeO	59.407
icsd_023425	CoGeNa ₂ O ₄	31.123	icsd_025657	ClOTi	59.411
icsd_040044	CoSSb	31.127	icsd_027010	BrOV	59.41
icsd_047101	MnNa ₅ O ₄	31.127	icsd_027092	BrCrO	59.409
icsd_071177	H ₂ KMnO ₅ P	31.125	icsd_028119	Br ₃ Ru	59.411
icsd_087325	HFeO ₂	31.127	icsd_059345	NaO ₅ V ₂	59.409
icsd_161305	Li ₂ MnO ₄ Si	31.125	icsd_069659	BrCrS	59.41
icsd_161306	FeLi ₂ O ₄ Si	31.123	icsd_074648	I ₃ Zr	59.407
icsd_420003	DFeO ₂	31.127	icsd_082689	CaO ₅ V ₂	59.41
icsd_670672	Li ₂ MnS ₄ Sn	31.127	icsd_088639	LiO ₅ V ₂	59.409
icsd_015009	AsFe	33.144	icsd_165626	BaCrS ₂	59.407
icsd_015057	FeP	33.144	icsd_173784	I ₃ Ti	59.407
icsd_015065	AsCo	33.148	icsd_195025	Fe ₂ OS ₂ Sr	59.411
icsd_023527	MnN ₂ Si	33.146	icsd_195027	Fe ₂ OSe ₂ Sr	59.411
icsd_023528	GeMnN ₂	33.146	icsd_260162	Br ₃ Tc	59.407
icsd_027117	FeNaO ₂	33.148	icsd_414041	Cl ₃ Ru	59.411
icsd_042445	AsV	33.148	icsd_428170	BaFe ₂ OS ₂	59.411
icsd_000284	MgO ₃ V	36.174	icsd_009965	CV ₂	60.42
icsd_001544	HFeO ₂	36.174	icsd_015522	Cl ₃ CuRb	60.422
icsd_002596	CrI ₂	36.174	icsd_020365	F ₂ Mn	60.422
icsd_052692	BaS ₃ V	36.176	icsd_023382	CrCsI ₃	60.417
icsd_068459	H ₂ CuO ₂	36.176	icsd_042979	Mn ₂ N	60.425
icsd_159030	CaIrO ₃	36.174	icsd_096077	Fe ₂ O ₃	60.424
icsd_050648	NbS ₂	38.189	icsd_006277	AgF ₂	61.436
icsd_004327	CuI ₂ O ₆	4.9	icsd_291504	MnS ₂	61.436
icsd_008010	FeI ₄ Rb ₂	4.9	icsd_000495	MnO ₃ Se	62.448
icsd_093022	O ₇ P ₂ V	4.9	icsd_000496	CoO ₃ Se	62.441
icsd_670113	CuFO ₂	4.7	icsd_000497	NiO ₃ Se	62.446
icsd_430557	Fe ₂ O ₃	41.211	icsd_000498	CuO ₃ Se	62.446
icsd_071339	NbSe ₂	42.221	icsd_000500	CoO ₃ Te	62.441
icsd_072198	Se ₂ Ta	42.221	icsd_000990	RuSb	62.444
icsd_095729	NbO	47.252	icsd_004063	Cl ₃ FeK	62.449
icsd_039871	HCSMnO ₁₀ P ₃	5.15	icsd_004064	Br ₃ FeK	62.441
icsd_059910	CsP ₂ S ₇ V	5.15	icsd_004404	CoF ₃ Na	62.448
icsd_075180	As ₂ FeLiO ₇	5.13	icsd_005418	CrP	62.443
icsd_084683	B ₂ BaCuO ₅	5.15	icsd_009008	F ₃ NaNi	62.441
icsd_091754	CrKP ₂ S ₇	5.15	icsd_015621	F ₃ MnNa	62.446
icsd_091756	KP ₂ S ₇ V	5.15	icsd_020228	MnO ₂	62.447
icsd_260893	CrCsP ₂ S ₇	5.15	icsd_022303	O ₂ V	62.448
icsd_025754	CuGeO ₃	51.294	icsd_023168	Cl ₃ MnTl	62.446
icsd_089669	CuO ₃ Si	51.294	icsd_023589	AsCr	62.443
icsd_015087	H ₄ Cl ₂ CuO ₂	53.328	icsd_024564	SV	62.449
icsd_009136	Cl ₄ MnNa ₂	55.358	icsd_026420	I ₃ MnTl	62.446
icsd_022046	GeMn ₂ O ₄	55.358	icsd_026422	FeI ₃ Tl	62.443
icsd_035130	Ca ₂ Mn ₂ O ₅	55.356	icsd_029338	CuO ₃ Te	62.448
icsd_035219	CaMnO _{2.5}	55.356	icsd_030413	AsFe	62.444
icsd_090183	Mn ₂ O ₅ Sr ₂	55.356	icsd_030450	BCo	62.449
icsd_400264	Cl ₄ Na ₂ Ti	55.353	icsd_031453	BaMnS ₂	62.449
icsd_005071	NiSe ₂	58.393	icsd_031820	F ₃ KMn	62.446
icsd_015027	FeP ₂	58.398	icsd_032710	Cl ₃ KMn	62.441
icsd_015467	Cl ₂ Cr	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 ₃ FeTl	62.443
icsd_034307	F ₂ Ni	58.398	icsd_038636	FNaNbO ₂	62.447
icsd_041123	H ₄ O ₄ V ₂	58.398	icsd_042441	Br ₃ KMn	62.446
icsd_048007	LiO ₂ Ru	58.398	icsd_042446	AsV	62.449
icsd_076826	CFe ₂	58.395	icsd_042577	AsRu	62.444
icsd_084619	O ₂ Ru	58.393	icsd_043248	FeP	62.444
icsd_155832	CrO ₂	58.398	icsd_043494	SiTi	62.445
icsd_172908	C ₂ H ₂ N ₄ Ni	58.398	icsd_048026	AsCo	62.449
icsd_236413	C ₂ H ₂ CoN ₄	58.397	icsd_051291	CaO ₃ Ru	62.441
icsd_419222	C ₂ H ₂ FeN ₄	58.393	icsd_052705	CaMnSb ₂	62.449
icsd_643441	MnS ₂	58.398	icsd_056697	O ₃ RuSr	62.447
icsd_001981	ClOV	59.41	icsd_066279	CrGaSe ₃	62.448
icsd_004086	ClCrO	59.409	icsd_068981	F ₃ FeNa	62.446
icsd_004202	Cu ₂ MgO ₃	59.409	icsd_074601	CrS ₃ Sb	62.447
icsd_010419	BrOTi	59.409	icsd_075469	Br ₃ FeIn	62.443
icsd_015094	CaCu ₂ O ₃	59.41	icsd_075470	Br ₃ InMn	62.446
icsd_015768	LiMnO ₂	59.407	icsd_076630	BMn	62.443
icsd_015769	MnNaO ₂	59.407	icsd_081056	CaO ₃ V	62.448

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_084866	CrSbSe ₃	62.446	icsd_670121	CuMgO ₂	67.506
icsd_084948	HMnO ₂	62.446	icsd_166017	As ₂ CaFe ₂	69.523
icsd_091273	N ₂ NiSr ₂	62.444	icsd_039528	Br ₇ FeSe	7.24
icsd_093161	CrTe	62.443	icsd_200680	CoGeNa ₂ O ₄	7.24
icsd_093835	FeO ₃ Tl	62.446	icsd_238234	FeGeLi ₂ S ₄	7.26
icsd_109041	DFeO ₂	62.446	icsd_238236	FeLi ₂ S ₄ Sn	7.26
icsd_109139	PRu	62.444	icsd_281242	I ₆ K ₂ Re	7.24
icsd_151925	ClMnS ₂ Sb	62.444	icsd_010038	BaMn ₂ O ₃	71.535
icsd_153239	CaMnO _{2.98}	62.448	icsd_015127	CuO ₃ Sr ₂	71.536
icsd_159433	CaIrO ₃	62.448	icsd_016216	Ca ₂ CuO ₃	71.536
icsd_160454	BiCrO ₃	62.446	icsd_024380	Cl ₂ OV	71.536
icsd_162895	BiFeO ₃	62.448	icsd_024381	Br ₂ OV	71.536
icsd_164775	CaO ₃ Rh	62.447	icsd_025001	CuLi ₂ O ₂	71.536
icsd_172156	BiClMnS ₂	62.444	icsd_025697	CsFeS ₂	71.535
icsd_172784	BrMnSbSe ₂	62.444	icsd_068700	FeLi ₄ N ₂	71.536
icsd_172790	CaMoO ₃	62.447	icsd_078012	AlF ₅ Fe	71.536
icsd_183450	O ₃ SrTc	62.441	icsd_251018	FeO ₃ Sr ₂	71.536
icsd_185586	CrInO ₃	62.441	icsd_633207	FeRbS ₂	71.535
icsd_193272	Bi ₃ Co	62.447	icsd_065453	K ₂ MnS ₂	72.542
icsd_196446	IrO ₃ Sr	62.448	icsd_065454	MnRb ₂ S ₂	72.542
icsd_237731	O ₃ OsSr	62.447	icsd_065455	Cs ₂ MnS ₂	72.542
icsd_237732	CaO ₃ Os	62.446	icsd_065456	K ₂ MnSe ₂	72.542
icsd_238293	BiMnO ₃	62.446	icsd_065457	MnRb ₂ Se ₂	72.542
icsd_238591	MnS	62.449	icsd_065458	Cs ₂ MnSe ₂	72.542
icsd_238684	CaFeOSe	62.444	icsd_065459	K ₂ MnTe ₂	72.542
icsd_238834	CrO ₃ Tl	62.447	icsd_065460	MnRb ₂ Te ₂	72.542
icsd_239321	HFeO ₂	62.444	icsd_065461	Cs ₂ MnTe ₂	72.542
icsd_245840	CaCrO ₃	62.448	icsd_067386	CoNa ₂ S ₂	72.542
icsd_247467	BiCoO ₃	62.446	icsd_067387	CoK ₂ S ₂	72.542
icsd_252431	NaO ₃ Os	62.448	icsd_067388	CoRb ₂ S ₂	72.542
icsd_261341	CaO ₃ Tc	62.448	icsd_067389	CoCs ₂ S ₂	72.542
icsd_425310	B ₂ Fe	62.443	icsd_067390	CoK ₂ Se ₂	72.542
icsd_643539	MnSb ₂ Sr	62.449	icsd_067391	CoRb ₂ Se ₂	72.542
icsd_652036	SeTi	62.449	icsd_067392	CoCs ₂ Se ₂	72.542
icsd_670832	CFe ₂ Si	62.447	icsd_624264	CoNa ₂ Se ₂	72.542
icsd_016217	CuO ₂ Sr	63.463	icsd_174205	MoO ₃ Sr	74.554
icsd_024885	HFeO ₂	63.459	icsd_183451	O ₃ SrTc	74.554
icsd_025524	CaIrO ₃	63.464	icsd_670124	CuO ₂ Pb	74.558
icsd_030603	BCr	63.461	icsd_670341	CaMnO ₃	74.559
icsd_036123	NiO ₂ Sr	63.463	icsd_006179	CCuO ₃	8.34
icsd_042952	BV	63.465	icsd_095439	Ca ₂ CoO ₃	8.34
icsd_054129	Cu ₄ O ₈	63.463	icsd_095440	CoO ₂	8.34
icsd_063228	BaS ₃ V	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 ₂ MnSe ₄	82.39
icsd_180910	O ₃ RuSr	63.457	icsd_052961	CoGa ₂ S ₄	82.39
icsd_187134	FeLiP	63.459	icsd_152909	Ga ₂ MnS ₄	82.39
icsd_192141	F ₃ NaNi	63.462	icsd_103995	Ga ₃ Ti ₂	10.44
icsd_192148	CoF ₃ Na	63.464	icsd_018307	O ₅ SV	85.59
icsd_251575	F ₃ FeNa	63.462	icsd_024894	MoO ₅ P	85.62
icsd_252147	BaCoOS	63.459	icsd_056181	HTi	13.69
icsd_613898	BFe	63.459	icsd_023081	BaFe ₂ S ₄	12.6
icsd_656056	Cs ₂ NiP ₂	63.464	icsd_033573	CuO ₆ Sr ₂ Te	87.75
icsd_658704	Bi ₂ Cs ₂ Ni	63.457	icsd_067826	IrNa ₄ O ₄	87.75
icsd_670104	BaCuO ₂	63.463	icsd_077697	O ₅ Ti ₄	12.6
icsd_670348	CaMnO ₃	63.464	icsd_174033	O _{1.25} Ti	12.6
icsd_001165	Cl ₄ Os	65.486	icsd_194696	MgO ₆ OsSr ₂	12.62
icsd_023265	Mn ₂ S ₄ Sn	65.486	icsd_238713	BaFe ₂ Se ₄	12.6
icsd_033865	Br ₄ Li ₂ Mn	65.486	icsd_001410	FeNa ₄ O ₃	9.39
icsd_073227	Cl ₄ CoLi ₂	65.486	icsd_010501	CoNa ₄ O ₃	9.39
icsd_082199	Br ₄ FeLi ₂	65.486	icsd_023174	CaCrF ₅	9.37
icsd_099041	Cu ₂ O ₃ Sr	65.483	icsd_069757	CuO	9.39
icsd_174117	CuF ₄ K ₂	65.486	icsd_169098	MoO ₅ P	9.37
icsd_174209	F ₇ KTi ₂	65.487	icsd_192515	BiFeO ₃	9.39
icsd_261512	Fe ₂ O ₅ Sr ₃	65.484	icsd_033768	FeNaO ₂	92.113
icsd_075515	BaCoS ₂	67.503	icsd_023173	F ₆ Li ₂ Mo	18.19
icsd_163555	FeSe	67.503	icsd_081589	H ₄ Cl ₂ CuO ₄ Pb ₂	99.167
icsd_163916	AsFFeSr	67.503	icsd_152276	O ₃ PbV	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 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_004189	CuO ₄ W	2.6	icsd_097745	MnO ₆ Sr ₂ W	14.75
icsd_030117	CuF ₆ Zr	2.4	icsd_098732	Ca ₂ CoO ₆ W	14.75
icsd_037027	Ba ₂ LaO ₆ Ru	2.4	icsd_098733	Ca ₂ NiO ₆ W	14.75
icsd_051506	AgF ₆ Ti	2.4	icsd_100793	Ba ₂ LaO ₆ Ru	14.79
icsd_078869	CuF ₁₁ NaZr ₂	2.4	icsd_160372	La ₂ NaO ₆ Ru	14.75
icsd_092852	CoLi ₂ O ₈ W ₂	2.4	icsd_170175	La ₂ NaO ₆ Os	14.75
icsd_092853	Li ₂ NiO ₈ W ₂	2.4	icsd_172591	FeO ₆ Sr ₂ Ta	14.75
icsd_092854	CuLi ₂ O ₈ W ₂	2.4	icsd_173491	CoO ₆ ReSr ₂	14.79
icsd_174140	Ba ₂ IrLaO ₆	2.4	icsd_203219	La ₂ LiMoO ₆	14.79
icsd_200533	CuFNbO ₃	2.4	icsd_238311	O ₆ OsSr ₂ Y	14.79
icsd_249777	Cd ₂ CuO ₈ P ₂	2.4	icsd_247998	Ca ₂ MnO ₆ Re	14.79
icsd_280299	H ₈ CdCl ₄ CuO ₄	2.4	icsd_291608	Ca ₂ O ₆ OsSc	14.75
icsd_159097	LaMnNaO ₆ W	4.7	icsd_413634	IrLa ₂ NaO ₆	14.79
icsd_237487	FeLaNaO ₆ W	4.7	icsd_414605	IrLa ₂ LiO ₆	14.79
icsd_238785	La ₂ Mn ₂ O ₁₂ Rb ₂ W ₂	4.7	icsd_416199	La ₂ LiO ₆ Os	14.79
icsd_238786	K ₂ La ₂ Mn ₂ O ₁₂ W ₂	4.7	icsd_099370	CoLaO ₃	15.89
icsd_238788	K ₂ Mn ₂ O ₁₂ W ₂ Y ₂	4.9	icsd_051698	CdO ₃ Ti	26.7
icsd_238789	La ₂ Mn ₂ Na ₂ O ₁₂ W ₂	4.7	icsd_236365	MnO ₃ Y	31.125
icsd_238791	Mn ₂ Na ₂ O ₁₂ W ₂ Y ₂	4.7	icsd_023822	FeO ₃ Y	33.148
icsd_238793	Mn ₂ O ₁₂ Rb ₂ W ₂ Y ₂	4.9	icsd_157925	HLaNiSn	62.444
icsd_068143	AgP ₂ Se ₆ V	5.13	icsd_057007	C ₂ CoY	38.189
icsd_425760	Ag ₂ FeS ₄ Si	7.26	icsd_617417	C ₂ CoLu	38.19
icsd_023476	CrNb ₂ Se ₄	8.34	icsd_617756	C ₂ FeLu	38.191
icsd_645393	Nb ₂ Se ₄ Ti	8.34	icsd_670125	CuO ₃ Pt	53.326
icsd_028909	CrO ₃ Y	10.46	icsd_073399	Cu ₂ La ₂ O ₅	55.359
icsd_150279	AuCrTe ₄	10.42	icsd_077943	CuLaO _{2.5}	55.359
icsd_035044	Cr ₂ Nb ₂ Se ₁₀	11.52	icsd_008146	LaO ₃ Ti	62.441
icsd_060759	CuF ₂ O ₃ W	11.5	icsd_008150	O ₃ TiY	62.446
icsd_066513	FeTaTe ₃	11.52	icsd_009938	CrLaO ₃	62.446
icsd_078041	F ₇ MnTiZr	11.52	icsd_014192	CrLaOS ₂	62.446
icsd_078042	F ₇ MnRbZr	11.53	icsd_016280	LaMnO ₃	62.447
icsd_084825	CoPZr ₂	11.53	icsd_020079	BCoRe	62.441
icsd_246091	Ca ₂ MnO ₆ Ta	11.54	icsd_027285	FeLuO ₃	62.446
icsd_252429	H ₃ ClCuO ₃ Zn	11.5	icsd_028255	FeLaO ₃	62.446
icsd_020661	FeSc ₂ Si ₂	12.61	icsd_039562	PVZr	62.444
icsd_077912	CoO ₆ Pb ₂ W	12.58	icsd_041893	B ₂ CoNb	62.441
icsd_174141	Ba ₂ IrLaO ₆	12.58	icsd_043260	FeO ₃ Y	62.446
icsd_427606	FeLa ₂ O ₂ Se ₂	12.62	icsd_049729	FePTa	62.443
icsd_617825	CFe ₂ Si ₂ Y 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 ₃ Y	62.447
icsd_008128	FeNbO ₄	13.67	icsd_063520	LaO ₃ V	62.446
icsd_015192	FeO ₄ W	13.68	icsd_076236	MnSiZr	62.444
icsd_015850	MnO ₄ W	13.68	icsd_076346	FeScSi	62.445
icsd_015851	CoO ₄ W	13.67	icsd_085141	CrO ₃ Sc	62.441
icsd_015852	NiO ₄ W	13.67	icsd_086280	FeHfP	62.443
icsd_036456	Ag _{0.5} Cr _{0.5} PS ₃	13.68	icsd_088387	CdO ₃ V	62.448
icsd_169005	CuO ₄ W	13.65	icsd_095577	O ₃ VY	62.446
icsd_170685	MnO ₄ Re	13.69	icsd_097805	GeMnY	62.444
icsd_202045	Ag _{0.5} PS ₃ V _{0.5}	13.68	icsd_109352	CrO ₃ Y	62.446
icsd_009390	CrO ₆ Ta ₂	14.79	icsd_155834	CoO ₃ Y	62.441
icsd_049500	O ₆ RuSr ₂ Y	14.75	icsd_160376	LuMnO ₃	62.447
icsd_051615	Ca ₂ MnO ₆ W	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 ₂ O ₆ Zn	14.79	icsd_260794	PtSiTi	62.445
icsd_079492	IrLa ₂ MgO ₆	14.79	icsd_409926	GePdTi	62.449
icsd_088152	IrO ₆ ScSr ₂	14.79	icsd_601849	CoLuSi	62.446
icsd_088153	Ba ₂ IrO ₆ Sc	14.75	icsd_601850	CoSnY	62.447
icsd_088154	IrO ₆ Sr ₂ Y	14.79	icsd_601861	CoGeLu	62.446
icsd_088155	Ba ₂ IrO ₆ Y	14.79	icsd_601862	CoLuSn	62.449
icsd_088156	Ba ₂ IrLaO ₆	14.79	icsd_610089	AsCoNb	62.441
icsd_088158	Ba ₂ IrLuO ₆	14.79	icsd_610502	AsFeNb	62.449
icsd_088522	La ₂ MgO ₆ Rh	14.75	icsd_610528	AsFeTa	62.443
icsd_088523	La ₂ O ₆ RhZn	14.79	icsd_613324	B ₂ CoTa	62.441
icsd_093880	AgCuO ₂	14.75	icsd_613388	BCoW	62.443
icsd_095517	FeO ₆ Sr ₂ W	14.79	icsd_623231	CoGaY	62.447
icsd_097487	La ₂ LiO ₆ Ru	14.75	icsd_623439	CoGeHf	62.449
icsd_097662	CoO ₆ Sr ₂ W	14.79	icsd_623611	CoGeTa	62.444

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_623685	CoGeZr	62.449	icsd_191362	CoLaO ₆ Sr ₂	71.536
icsd_623786	CoHfP	62.443	icsd_191363	CoO ₆ Sr ₂ Zr	71.536
icsd_624322	CoNbSi	62.449	icsd_191629	La ₂ NiO ₆ Zr	71.536
icsd_624621	CoPSc	62.446	icsd_191630	HfLa ₂ NiO ₆	71.536
icsd_624977	CoScSn	62.446	icsd_238076	Ag ₂ Ba ₂ CoO ₂ Se ₂	71.536
icsd_625144	CoSiZr	62.446	icsd_623793	Co ₂ HfSi ₂	71.535
icsd_626229	CrLaSe ₃	62.443	icsd_625135	Co ₂ Si ₂ Zr	71.535
icsd_626529	CrPZr	62.444	icsd_633666	Fe ₂ Si ₂ Zr	139.536
icsd_632166	FeGeZr	62.443	icsd_634333	Ga ₄ HfV ₂	71.535
icsd_632827	FeNbSi	62.445	icsd_635647	Ga ₄ V ₂ Zr	69.523
icsd_633568	FeSiTa	62.443	icsd_051014	MnO ₈ Re ₂	2.4
icsd_633674	FeSiZr	62.444	icsd_051015	CoO ₈ Re ₂	2.4
icsd_648877	PdSiTi	62.445	icsd_164936	CrLaO ₆ Te	15.87
icsd_085926	LaMnSi ₂	63.465	icsd_030116	CuF ₆ Zr	148.17
icsd_195899	AsCo ₂ LaN	63.461	icsd_152678	Ba ₂ IrLaO ₆	2.4
icsd_632049	FeGe ₂ La	63.461	icsd_155549	Ba ₂ LaO ₆ Ru	148.17
icsd_632434	FeLaSi ₂	63.459	icsd_262503	C ₆ Ag ₃ KMnN ₆	5.15
icsd_670675	AlTi ₂ Zr	63.465	icsd_024797	AgCrS ₂	8.32
icsd_009389	OTi ₂ Zr	65.483	icsd_024799	AgCrSe ₂	8.32
icsd_035337	MnO ₆ Pt ₃	65.486	icsd_084639	CrN ₂ W	160.67
icsd_035338	CoO ₆ Pt ₃	65.485	icsd_605002	AgCrTe ₂	8.32
icsd_180434	AsFeLaO	67.503	icsd_605619	AgNiTe ₂	8.32
icsd_068795	BaNiO ₅ Y ₂	71.536	icsd_173552	C ₆ Ag ₃ FeN ₆	12.58
icsd_613131	B ₄ Co ₄ La	13.67	icsd_032731	CdCoF ₆ Li	15.87
icsd_009294	NiO ₆ Sr ₂ W	12.62	icsd_039666	Cl ₆ FeZr	15.87
icsd_078677	FeO ₆ Sr ₂ W	12.62	icsd_039817	Cl ₆ FeHf	163.81
icsd_095518	Ba ₂ FeO ₆ W	12.62	icsd_240281	Ba ₃ NiO ₉ Ta ₂	12.58
icsd_150702	FeO ₆ ReSr ₂	12.62	icsd_004149	AgCrO ₂	166.101
icsd_190593	CoO ₆ Sr ₂ W	12.62	icsd_031919	AgFeO ₂	166.101
icsd_192327	CoNbO ₆ Sr ₂	12.62	icsd_099369	CoLaO ₃	15.85
icsd_262352	Co _{0.5} O ₃ Re _{0.5} Sr	12.62	icsd_042650	NbS ₂ V _{0.333}	20.31
icsd_075318	BBaCuLaO ₅	100.174	icsd_042687	FeNb ₃ S ₆	20.31
icsd_042534	Ag ₂ FeS ₄ Sn	23.51	icsd_624304	CoNb ₃ Se ₆	20.34
icsd_192470	AgFe ₂ GaTe ₄	121.327	icsd_626392	CrNb ₃ S ₆	20.34
icsd_056263	AgFeS ₂	43.226	icsd_626398	CrNb ₃ Se ₆	20.34
icsd_051261	ClCuLaO ₇ Ta ₂	47.252	icsd_626633	CrS ₆ Ta ₃	20.34
icsd_064639	Ba ₂ Cu ₂ LaO ₈ Ta	123.347	icsd_626727	CrSe ₆ Ta ₃	20.34
icsd_074164	Cu ₂ O ₇ Sr ₂ TIY	123.347	icsd_633323	FeS ₆ Ta ₃	20.33
icsd_075720	Ba ₂ CuHgO ₄	123.345	icsd_643472	MnS ₆ Ta ₃	20.34
icsd_075725	Ba ₂ CaCu ₂ HgO ₆	123.347	icsd_645098	Nb ₃ NiSe ₆	182.182
icsd_088032	ClCuLaNb ₂ O ₇	47.252	icsd_645331	Nb ₃ S ₆ Ti	20.33
icsd_088033	BrCuLaNb ₂ O ₇	47.252	icsd_645338	Nb ₃ S ₆ V	20.33
icsd_016496	CrNNb	59.407	icsd_651970	Se ₆ Ta ₃ V	182.183
icsd_080798	ClFeO ₄ W	67.503	icsd_080029	MnN ₂ W	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 ₂ Nb	67.503	icsd_042061	CrGeNb	38.191
icsd_237385	AsCrLaO	59.407	icsd_054566	Bi ₂ CoHf ₆	38.189
icsd_262356	As ₂ Co ₂ O ₆ Sc ₂ Sr ₄	67.506	icsd_090081	FeSc ₆ Te ₂	38.191
icsd_262357	Co ₂ O ₆ P ₂ Sc ₂ Sr ₄	59.407	icsd_096247	FeSb ₂ Sc ₆	38.191
icsd_624027	CoLaSi	67.503	icsd_150575	Al ₂ CoZr ₆	38.191
icsd_657914	FeLaSb ₂	67.503	icsd_041460	Co ₆ Ge ₆ Zr	191.241
icsd_657919	CoLaSb ₂	67.503	icsd_155117	Ge ₆ HfMn ₆	65.483
icsd_002575	O ₆ V ₂ W	136.502	icsd_604198	FePb ₃ Zr ₅	63.464
icsd_015306	CrO ₆ Ta ₂	58.398	icsd_002786	AgFeO ₂	194.268
icsd_020314	Cr ₂ O ₆ W	136.502	icsd_057984	AlMnPt	63.462
icsd_023600	O ₆ Ta ₂ V	136.499	icsd_080373	C ₂ CrSc	194.266
icsd_040337	FeO ₆ Ta ₂	58.398	icsd_081488	FeN ₂ W	63.462
icsd_061198	NiO ₆ Ta ₂	136.501	icsd_156263	GaPtTi	63.462
icsd_083367	CuO ₆ Ta ₂	136.499	icsd_163350	AlPtTi	63.462
icsd_166673	CoO ₆ Ta ₂	58.398	icsd_164891	Ge ₃ LaV	63.462
icsd_173874	Cr ₂ O ₆ Re	136.501	icsd_172878	Ag ₃ Ni ₂ O ₄	63.461
icsd_075384	CrF ₆ Nb	69.524	icsd_180888	AgCoO ₂	63.464
icsd_092989	AsTiZr	71.536	icsd_261608	AgCoO ₂	63.461
icsd_168330	Co ₂ La ₂ O ₃ Se ₂	71.536	icsd_103606	FePtSb	19.27
icsd_191357	CrO ₆ Sr ₂ Zr	71.536	icsd_181053	Cd _{0.75} Cr _{0.25} Te	160.67
icsd_191358	CrHfO ₆ Sr ₂	71.536	icsd_181055	Cd _{0.25} Cr _{0.75} Te	160.67
icsd_191359	O ₆ Sr ₂ VZr	71.536	icsd_186189	Cr _{0.25} TeZn _{0.75}	111.255
icsd_191360	HfO ₆ Sr ₂ V	71.536	icsd_054465	AuMnSn	44.231
icsd_191361	CoO ₆ Sr ₂ Y	71.536	icsd_057421	MnPtSb	160.67

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_083928	FeNbSb	119.319	icsd_030379	CuMnO ₂	12.62
icsd_102552	CoNbSn	44.231	icsd_035634	FeS ₄ V ₂	12.62
icsd_104955	MnPtSn	160.67	icsd_040850	MnO ₆ V ₂	12.62
icsd_105220	NbRhSn	119.319	icsd_041802	Cl ₃ CrCs	12.62
icsd_107129	CoNbSb	119.319	icsd_043042	Cr ₂ FeSe ₄	12.62
icsd_108317	CoSbZr	44.231	icsd_043412	Te ₄ Ti ₃	12.58
icsd_190997	MnSc ₂ Si	160.67	icsd_052510	Te ₄ V ₃	12.62
icsd_190999	GeMnSc ₂	44.231	icsd_099989	Co ₃ Se ₄	12.62
icsd_671364	BiMnPt	160.67	icsd_150462	MnO ₂	12.62
icsd_028925	LaO ₃ V	166.101	icsd_169764	CrF ₃ K	12.62
icsd_028930	CrLaO ₃	123.345	icsd_172782	BrMnS ₂ Sb	12.62
icsd_029118	FeLaO ₃	166.101	icsd_188911	CoO ₆ V ₂	12.62
icsd_076057	Mn ₃ NPd	166.101	icsd_193869	Ni _{0.5} Se ₂ Ti	12.62
icsd_422858	CdCo ₃ N	65.486	icsd_195677	BiBrFeS ₂	12.58
icsd_052994	Co ₂ GeZn	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 ₃ O ₈ P ₂	2.4	icsd_601038	CoCr ₂ Se ₄	12.62
icsd_024284	B ₂ Co ₂ O ₅	2.6	icsd_625012	CoSe ₄ V ₂	12.58
icsd_028151	CuO ₆ V ₂	2.4	icsd_625931	Cr ₂ FeS ₄	12.62
icsd_039439	CuMoO ₄	2.6	icsd_626279	Cr ₂ MnS ₄	12.58
icsd_039887	H ₂ CuO ₅ Se	2.4	icsd_626299	Cr ₂ MnSe ₄	12.62
icsd_043508	AsFeS	2.6	icsd_626579	CrRh ₂ Te ₄	12.62
icsd_050506	CuF ₆ Mo	2.4	icsd_626640	Cr ₂ S ₄ Ti	12.62
icsd_050507	CrF ₆ Mo	2.4	icsd_626896	Cr ₂ Te ₄ Ti	12.62
icsd_059720	BiMnO ₅ V	2.6	icsd_626901	Cr ₂ Te ₄ V	12.62
icsd_063057	As ₂ Cu ₃ O ₈	2.4	icsd_633504	FeSe ₄ Ti ₂	12.62
icsd_064660	CuF ₆ Pt	2.4	icsd_061078	MnMoO ₄	13.67
icsd_068184	H ₂ CuO ₅ S	2.4	icsd_081060	MoNiO ₄	13.67
icsd_087710	H ₂ FeO ₅ V	2.6	icsd_081061	CoMoO ₄	13.68
icsd_095571	LiMoS ₂	2.6	icsd_411172	K ₂ Mn ₃ S ₄	13.67
icsd_099499	C ₆ CuFeK ₂ N ₆	2.4	icsd_054919	LaMnO ₃	14.79
icsd_100442	As ₂ Fe ₄ O ₁₁	2.6	icsd_073900	LaO ₃ V	14.75
icsd_167202	CoFLiO ₄ S	2.4	icsd_079494	IrLa ₂ NiO ₆	14.75
icsd_167608	HFeLiO ₅ P	2.4	icsd_079495	CoIrLa ₂ O ₆	14.75
icsd_180390	FFeO ₄ S	2.4	icsd_088043	NiO ₃ Y	14.79
icsd_180391	FLiNiO ₄ S	2.4	icsd_089955	Ca ₂ FeMoO ₆	14.75
icsd_184601	FLiO ₄ PV	2.4	icsd_092051	LuNiO ₃	14.79
icsd_189335	MoO ₆ Sr ₂ Ti	2.4	icsd_092336	CaFeO ₃	14.79
icsd_193472	Cu ₃ Nb ₂ O ₈	2.4	icsd_095578	O ₃ VY	14.75
icsd_246513	BaMn ₂ O ₆ Y	2.4	icsd_096085	CuGeO ₃	14.75
icsd_246811	B ₂ Fe ₂ O ₅	2.6	icsd_096120	La ₂ NiO ₆ Ru	14.79
icsd_260257	NiO ₁₀ Te ₂ V ₂	2.4	icsd_097744	MnMoO ₆ Sr ₂	14.75
icsd_416823	HCoO ₅ PZn	2.4	icsd_151888	Mn _{0.5} Ni _{0.5} O ₃ Y	14.79
icsd_099699	BaMn ₂ O ₆ Y	3.3	icsd_152444	Ca ₂ NiO ₆ Os	14.79
icsd_036263	MoO ₂	4.9	icsd_153857	Bi ₂ MnNiO ₆	14.75
icsd_084868	CaCuO ₂	4.7	icsd_163761	La ₂ MnO ₆ V	14.79
icsd_192247	CoY ₃	4.9	icsd_181147	FeMn ₂ O ₆ Sb	14.79
icsd_021067	CuO ₆ V ₂	5.13	icsd_186428	La ₂ MnNiO ₆	14.79
icsd_046003	CoO ₆ V ₂	5.15	icsd_188476	Cr _{0.5} Mn _{0.5} O ₃ Y	14.75
icsd_060512	DV ₂	8.34	icsd_188982	CoMnO ₆ Y ₂	14.75
icsd_069869	CaClFeO ₂	8.32	icsd_191374	CrMnO ₆ Y ₂	14.79
icsd_001503	O ₂ V	10.46	icsd_192122	CoLa ₂ O ₆ Ti	12.62
icsd_081569	Fe ₂ O ₁₂ Se ₄ Sr	10.42	icsd_192872	MnNiO ₆ Y ₂	14.79
icsd_089471	O ₂ V	10.46	icsd_195628	FeMn ₂ O ₆ Re	14.75
icsd_100696	D ₂ FeTi	10.45	icsd_237528	In ₂ MnNiO ₆	14.79
icsd_601978	H ₂ FeTi	10.45	icsd_238148	Ca ₂ FeO ₆ Os	14.75
icsd_000901	AsClCu ₂ O ₄	11.54	icsd_251022	MnO ₃ Sc	14.75
icsd_000902	AsClCo ₂ O ₄	11.5	icsd_251832	MnNiO ₆ Sc ₂	14.79
icsd_051677	H ₃ ClCu ₂ O ₃	11.54	icsd_252567	Mn ₃ O ₆ Re	14.79
icsd_065346	ClFeLiMoO ₄	11.52	icsd_093795	CoMoO ₆ Te	18.19
icsd_162834	BiFeO ₃	11.55	icsd_163978	MnMoO ₆ Te	18.19
icsd_240499	BrOTi	11.54	icsd_037026	FeNaS ₂	23.51
icsd_415798	Cl ₂ Co ₂ O ₃ Te	11.5	icsd_015105	LiMnO ₂	59.407
icsd_657748	O ₂ Ti	11.54	icsd_001898	NaO ₅ V ₂	31.125
icsd_002225	Cl ₃ CrRb	12.62	icsd_042490	Cu ₂ GeMnS ₄	31.127
icsd_015043	Fe ₃ Se ₄	12.62	icsd_088640	LiO ₅ V ₂	31.125
icsd_016722	Cr ₃ S ₄	12.62	icsd_193986	Cu ₂ MnS ₄ Si	31.125
icsd_016884	Cr ₂ NiS ₄	12.62	icsd_627355	Cu ₂ FeS ₄ Si	31.123
icsd_024566	S ₄ V ₃	12.62	icsd_627741	Cu ₂ GeMnSe ₄	31.127

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_628396	Cu ₂ MnSe ₄ Si	31.127	icsd_090827	Cu ₂ FeS ₄ Sn	3.3
icsd_041646	Ba ₂ Cu ₃ O ₇ Y	47.253	icsd_027315	MoO ₅ V	85.62
icsd_081167	Ba ₂ Cu ₃ LaO ₇	47.253	icsd_015451	Te ₄ Ti ₅	87.78
icsd_161972	Ba ₂ Cu ₃ LuO ₇	47.253	icsd_024563	S ₄ V ₅	12.62
icsd_164175	BaFe ₂ O ₅ Y	51.291	icsd_042881	Te ₄ V ₅	12.62
icsd_171434	BaCo ₂ O ₅ Y	51.296	icsd_055075	Se ₄ Ti ₅	87.79
icsd_658677	Co ₂ InY	51.295	icsd_098191	MoNiO ₆ Sr ₂	12.62
icsd_020933	Fe ₂ HfSi ₂	57.38	icsd_150701	FeMoO ₆ Sr ₂	12.62
icsd_087157	Fe ₂ ScSi ₂	57.381	icsd_152440	NiO ₆ OsSr ₂	12.62
icsd_033996	CoCu ₂ O ₃	59.41	icsd_153544	CoMoO ₆ Sr ₂	12.62
icsd_005432	CoMnSi	62.446	icsd_187669	MnMoO ₆ Sr ₂	12.62
icsd_020461	BCoMo	62.443	icsd_191960	Ba ₂ CuO ₆ Os	12.62
icsd_041918	GeMnNi	62.447	icsd_192904	Ca ₂ MnO ₆ Ti	12.62
icsd_043896	AsCoRh	62.444	icsd_236435	CoO ₆ OsSr ₂	12.62
icsd_044052	AsRhTi	62.445	icsd_245819	CuO ₆ OsSr ₂	12.62
icsd_052968	CoGeMn	62.447	icsd_250818	IrNiO ₆ Sr ₂	12.62
icsd_053283	CuGeTi	62.441	icsd_652166	Se ₄ V ₅	12.62
icsd_067558	Cu ₂ NaO ₂	62.444	icsd_067978	BaCuFeO ₅ Y	25.59
icsd_071221	Cu ₂ LiO ₂	62.444	icsd_167073	F ₆ LiMnV	102.19
icsd_072411	CuMnP	62.443	icsd_202705	F ₆ Fe ₂ Li	34.158
icsd_072413	AsCuMn	62.444	icsd_291413	MnMoO ₆ Te	18.19
icsd_087197	CuSiTi	62.447	icsd_063423	Ba ₂ Cu ₃ O ₆ Y	115.285
icsd_098405	MoPRu	62.446	icsd_026721	Cu ₂ FeS ₄ Sn	42.221
icsd_107965	AsRhV	62.443	icsd_042489	Cu ₂ MnS ₄ Sn	121.331
icsd_151867	CrFeP	62.444	icsd_047165	Cu ₂ FeGeS ₄	23.51
icsd_158732	MnO ₃ Ti	62.446	icsd_085126	Cu ₂ FeSe ₄ Sn	23.51
icsd_165243	FeNiSi	62.441	icsd_099292	CoCu ₂ S ₄ Si	23.51
icsd_165248	CoCrSi	62.449	icsd_099293	CoCu ₂ GeS ₄	121.331
icsd_165254	NiSiV	62.449	icsd_099294	CoCu ₂ S ₄ Sn	121.331
icsd_165255	CrNiSi	62.446	icsd_099296	CoCu ₂ Se ₄ Sn	121.331
icsd_185418	MnO ₃ V	62.441	icsd_155904	Cu ₂ MnSe ₄ Sn	121.331
icsd_187466	O ₃ Ti ₂	62.446	icsd_160047	CuFe ₂ InSe ₄	121.327
icsd_246514	FeO ₃ Ti	62.445	icsd_627313	Cu ₂ FeGeSe ₄	42.221
icsd_260758	Fe ₃ N	62.449	icsd_627368	Cu ₂ FeSe ₄ Si	23.51
icsd_610884	AsMnNi	62.446	icsd_015521	ClFe ₃ O ₈ Pb ₄	65.486
icsd_611086	AsNiTi	62.443	icsd_098113	Ba ₂ Cu ₃ LuO ₆	123.347
icsd_611097	AsNiV	62.443	icsd_187030	AlTi	53.334
icsd_614129	BFe ₂ Ni	62.446	icsd_004054	F ₃ KMn	55.358
icsd_622955	CoFeP	62.441	icsd_059553	In ₄ Ti 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 ₃ Sn ₂	62.447	icsd_049516	ClFeMoO ₄	67.503
icsd_632538	FeMnP	62.449	icsd_084962	CrCuO ₃ SSr ₂	59.407
icsd_632646	FeMoP	62.444	icsd_084963	CuFeO ₃ SSr ₂	67.503
icsd_633116	FePV	62.443	icsd_088949	BaMn ₂ O ₅ Y	129.419
icsd_637435	GeNiV	62.444	icsd_169992	Ca ₂ CuFeO ₃ S	59.407
icsd_643093	MnNiP	62.449	icsd_169993	Ca ₂ CuFeO ₃ Se	59.407
icsd_646165	NiPTi	62.447	icsd_423230	AsCuMn	59.407
icsd_646176	NiPV	62.443	icsd_191628	La ₂ NiO ₆ Ti	71.536
icsd_670836	CFe ₂ Ti	62.444	icsd_670534	CoFeLa ₂ O ₆	139.537
icsd_025761	CAsV ₃	63.465	icsd_670535	FeIrLa ₂ O ₆	139.537
icsd_079258	B ₃ V ₂	63.465	icsd_200593	HNi ₂	1.1
icsd_180767	Ni ₃ S ₂	63.459	icsd_162263	Bi ₂ FeO ₆ Ti	1.1
icsd_189439	Fe ₂ O ₃	63.464	icsd_246426	Bi ₂ CrFeO ₆	146.1
icsd_246516	FeO ₃ Ti	63.459	icsd_191591	CsFeMo ₂ O ₈	2.4
icsd_601350	B ₃ Cr ₂	63.461	icsd_194588	Ag ₂ FeO ₈ RbV ₂	2.4
icsd_610970	AsNV ₃	63.459	icsd_194590	Ag ₂ FeKO ₈ V ₂	2.4
icsd_617981	CGeV ₃	63.459	icsd_245666	FeMo ₂ O ₈ Rb	2.4
icsd_618621	CPV ₃	63.461	icsd_408193	Ag ₂ BaMnO ₈ V ₂	2.4
icsd_634723	GaNv ₃	63.461	icsd_417823	C ₆ Mn ₂ N ₆ Ru	147.15
icsd_637164	GeNV ₃	63.465	icsd_417824	C ₆ FeMn ₂ N ₆	147.15
icsd_644620	NPV ₃	63.465	icsd_417825	C ₆ Mn ₂ N ₆ Os	147.15
icsd_050089	Cu ₆ O ₁₀ Sr ₄	65.485	icsd_429825	BaLi ₂ MnO ₈ V ₂	2.4
icsd_065881	BaCu ₃ O ₄	65.485	icsd_015988	NiO ₃ Ti	2.6
icsd_044175	B ₄ Co ₂ Mo	71.535	icsd_016548	CoO ₃ Ti	2.4
icsd_188992	GaMnNi ₂	71.536	icsd_024790	FeO ₃ Ti	2.6
icsd_416904	Cu ₃ O ₅ Sr ₂	71.536	icsd_031853	MnNiO ₃	2.4
icsd_670346	CaMnO ₃	71.536	icsd_031854	CoMnO ₃	148.19
icsd_036535	Cu ₂ O ₂ Tl	74.558	icsd_044407	MnO ₃ Ti	2.6
icsd_069870	Ca ₂ ClFeO ₃	35.167	icsd_087943	F ₃ Ni	2.4

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.201765	CoLaO ₃	2.4	icsd.054259	NiSnTi	44.231
icsd.029133	CoF ₃	5.13	icsd.054343	MnRhSb	44.231
icsd.029134	F ₃ Rh	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 ₄ S ₈	8.32	icsd.182484	CrNiSb	44.231
icsd.036563	GaMo ₄ Se ₈	8.32	icsd.184947	GeMn ₂	160.67
icsd.036564	AlMo ₄ S ₈	8.32	icsd.189702	InTi ₂	44.231
icsd.158199	GaS ₈ V ₄	8.32	icsd.191682	CoTeV	119.319
icsd.195253	GaSe ₈ V ₄	8.32	icsd.191684	CoCrTe	119.319
icsd.039428	Cl ₃ Ti	15.87	icsd.191687	FeMnTe	44.231
icsd.031342	Li _{0.33} S ₂ Ti	12.62	icsd.670784	AlCrVZr	160.67
icsd.062661	Mn ₃ Nb ₆ O ₁₁	12.58	icsd.670785	AlCrHfV	160.67
icsd.073874	Li ₂ NiO ₂	165.96	icsd.670787	CrGaVZr	160.67
icsd.100782	K ₃ O ₈ V ₃	12.62	icsd.670788	CrGaHfV	44.231
icsd.153864	FeKMo ₂ O ₈	12.62	icsd.670790	CrInVZr	44.231
icsd.155025	Fe ₂ In ₂ Se ₅	12.58	icsd.670791	CrHfInV	160.67
icsd.202907	CsMo ₂ O ₈ V	12.62	icsd.670792	CrScSiV	44.231
icsd.245665	FeMo ₂ O ₈ Rb	12.62	icsd.670793	CrGeScV	44.231
icsd.260887	CsFeMo ₂ O ₈	12.58	icsd.670794	CrScSnV	160.67
icsd.429824	BaLi ₂ MnO ₈ V ₂	12.58	icsd.670795	CrSiVY	160.67
icsd.429826	BaCoNa ₂ O ₈ V ₂	12.58	icsd.670796	CrGeVY	44.231
icsd.429827	BaFeNa ₂ O ₈ V 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 ₂ Si	160.67
icsd.670109	CoCuO ₂	12.62	icsd.051984	InMnNi ₂	166.101
icsd.068847	FeS	36.176	icsd.053555	Fe ₂ SiV	166.101
icsd.042735	CoSiTi	189.223	icsd.053706	GeMnRh ₂	166.101
icsd.042943	CoGeTi	38.191	icsd.057807	AlFe ₂ Mo	166.101
icsd.623085	CoGaHf	38.189	icsd.057976	AlMnNi ₂	166.101
icsd.637069	GeMnRh	38.191	icsd.058071	AlNi ₂ V	166.101
icsd.648274	P ₃ V ₅	63.461	icsd.076227	Mn ₃ Si	166.101
icsd.066546	CuFeO ₂	194.268	icsd.102437	CoGa ₂ Mn	166.101
icsd.081489	MnMoN ₂	63.457	icsd.102531	Co ₂ MnSn	166.101
icsd.082065	CrCuO ₂	194.268	icsd.103803	GaMnNi ₂	166.101
icsd.181348	AlN ₃ V ₄	63.461	icsd.104936	MnPbRh ₂	166.101
icsd.409451	CoCrGe	63.462	icsd.104964	MnRh ₂ Sn	166.101
icsd.624219	CoMoP ₂	194.268	icsd.155336	Ga ₄ Mn ₄ Ni ₈	166.101
icsd.629351	Cu ₃ Te ₄ V	111.255	icsd.186057	Fe ₂ GeTi	71.535
icsd.042978	CuMnSb	44.231	icsd.186061	Fe ₂ MnSi	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 [62, 63, 65–84]. 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 S50. 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 $\text{CsV}_2\text{S}_2\text{O}$ in section V A.

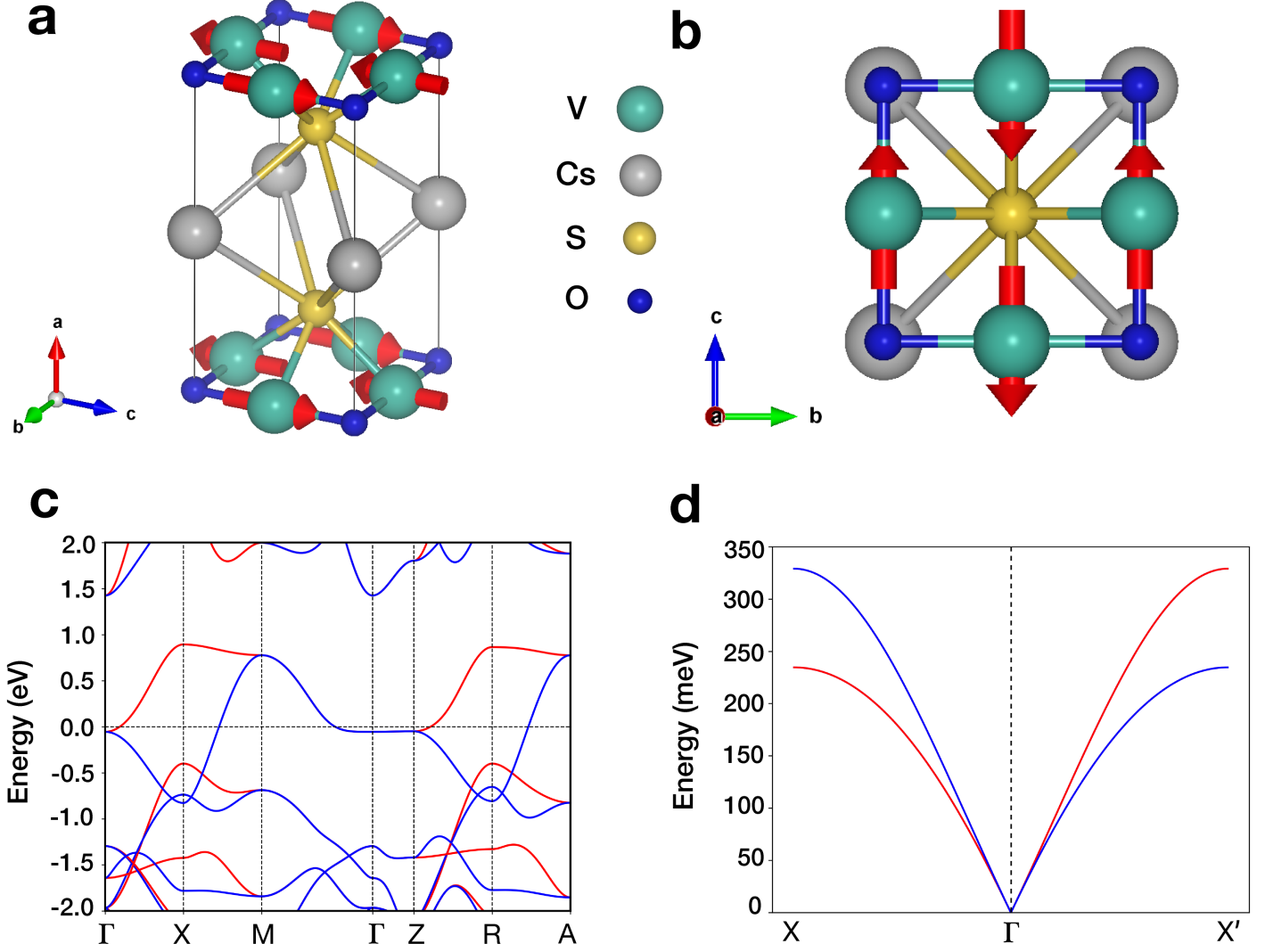
A. Representative material of Altermagnetism $\text{CsV}_2\text{S}_2\text{O}$ Altermagnetism $\text{CsV}_2\text{S}_2\text{O}$ 

FIG. S5. (a)(b) Crystal structure of $\text{CsV}_2\text{S}_2\text{O}$. (c) Electron band splitting of $\text{CsV}_2\text{S}_2\text{O}$ 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.

$\text{CsV}_2\text{S}_2\text{O}$ crystallizes in space group $P4/mmm$ (No. 123) with magnetic ions occupying the $1b$ Wyckoff positions, as shown in Fig. S5(a). It exhibits a pronounced altermagnetic spin splitting along high-symmetry paths [Fig. S5(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 [85] and approximately 2 meV in MnTe [86]. Based on the magnetic force theorem and linear-response calculations [87–89], 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. S5(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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