Algorithm for deriving magnetic space-group information

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(Received 0 XXXXXX 0000; accepted 0 XXXXXX 0000)

Abstract

A crystal symmetry search is crucial for computational crystallography and materials science. Although algorithms and implementations for the crystal symmetry search have been developed, their extension to magnetic space groups (MSGs) remains limited. In this paper, algorithms for determining magnetic symmetry operations of magnetic crystal structures, identifying magnetic space-group types of given MSGs, and symmetrizing the magnetic crystal structures using the MSGs are presented. The determination of magnetic symmetry operations is numerically stable and is implemented with minimal modifications from the existing crystal symmetry search. Magnetic space-group types are identified by combining space-group type identification and the use of affine normalizers. Point coordinates and magnetic moments of the magnetic crystal structures are symmetrized by projection operators for the MSGs.
1. Introduction

A crystal symmetry search and the standardization of crystal structures play crucial roles in computational materials science. For example, symmetry operations are required in irreducible representations of electronic states (Gao et al., 2021), band paths (Hinuma et al., 2017), phonon calculations (Togo & Tanaka, 2015; Togo et al., 2015), a random structure search (Fredericks et al., 2021), and crystal structure description (Ganose & Jain, 2019). Moreover, the standardization of crystal structures is indispensable for comparing crystal structures in different settings and analyzing magnetic crystal structures in high-throughput first-principles calculations (Horton et al., 2019).

Owing to the development of a computer-friendly description of space groups (Hall, 1981; Shmueli et al., 2010) and algorithms (Opgenorth et al., 1998; Grosse-Kunstleve, 1999; Grosse-Kunstleve & Adams, 2002; Eick & Souvignier, 2006), we can automatically perform the crystal symmetry search nowadays. For example, SPGLIB implements the symmetry-search algorithm and an iterative method to robustly determine crystal symmetries (Togo & Tanaka, 2018), which one of the authors has developed and maintained.

On the other hand, algorithms and implementations for magnetic space groups (MSGs) (Litvin, 2016) remains limited. MSGs are essential when we consider time-reversal operations or magnetic crystal structures. To the best of our knowledge, existing implementations only partly provide MSG functionalities. AFLOW-SYM (Hicks et al., 2018) proposed and implemented a robust space-group analysis algorithm; however, it does not seem to support MSGs yet. IDENTIFY MAGNETIC GROUP (Perez-Mato
et al., 2015) in the Bilbao Crystallographic Server (Aroyo et al., 2011) can identify MSGs from magnetic symmetry operations; however, the determination of magnetic symmetry operations from magnetic crystal structures is not supported. FINDSYM (Stokes & Hatch, 2005; Stokes et al., 2022) supports the determination of magnetic symmetry operations and the identification of MSGs; however, the source code is not freely available.

Here, we present algorithms for determining magnetic symmetry operations of given magnetic crystal structures, identifying magnetic space-group types of given MSGs, and symmetrizing the magnetic crystal structures on the basis of the determined MSGs. Note that the implementation of these algorithms is virtually unattainable without recent development in crystallography: Litvin (2014) provided extensive tables for the 1651 MSGs. Magnetic Hall symbols (González-Platas et al., 2021) and unified (UNI) MSG symbols (Campbell et al., 2022) have been developed to represent MSGs or magnetic space-group types unambiguously, which are based on BNS symbols (Belov et al., 1957; Bradley & Cracknell, 2009). In this paper, we use the magnetic Hall symbols to tabulate MSGs for each magnetic space-group type. The implementation is distributed under the BSD 3-clause license in SPGLIB v2.0.2.

This paper is organized as follows. In Sec. 2 we recall the mathematical structures of MSGs and present definitions and terminology for describing MSGs. In Sec. 3 we provide an algorithm for determining magnetic symmetry operations of a given magnetic crystal structure on the basis of equivalence relationships between sites in the magnetic crystal structure. In Sec. 4 we provide an algorithm to identify a magnetic space-group type of the determined MSG and to find a transformation from the determined MSG to a standardized one. In Sec. 5 we provide an algorithm to symmetrize point coordinates and magnetic moments of the magnetic crystal structure from the determined MSG.
2. Definitions

Before we discuss algorithms for MSGs and magnetic crystal structures, we describe definitions and terminology for MSGs. In Sec. 2.1, we define MSGs and derived space groups, which are essential in identifying a magnetic space-group type. In Sec. 2.2, we define equivalence relationships between MSGs. In Sec. 2.3, we mention BNS symbols and their settings, which specify representatives of MSGs, and we use them to standardize given MSGs. Finally, in Sec. 2.4, we give examples of actions of magnetic symmetry operations for collinear and non-collinear magnetic moments.

2.1. MSG and its construct type

Let $S$ be a subgroup of the three-dimensional Euclidean group $E(3)$. A \textit{symmetry operation} $(W, w) \in S$ acts on point coordinates $x$ as

$$(W, w)x = Wx + w,$$

where we call $W$ as a \textit{linear part} and $w$ as a \textit{translation part} of the symmetry operation. A \textit{translation subgroup} of $S$ is a subgroup of $S$ whose linear parts of symmetry operations are identity matrices:

$$T(S) := \{(E, t) \mid (E, t) \in S\},$$

where $E$ represents the identity matrix. The subgroup $S$ is called a \textit{space group} when its translation subgroup is generated from three independent translations. We write a \textit{point group} of $S$ as

$$P(S) := \{W \mid \exists w \in \mathbb{R}^3, (W, w) \in S\}.$$

We consider a \textit{time-reversal operation} $1'$ and call an index-two group generated from $1'$ as a \textit{time-reversal group} $\{1, 1'\} (\cong \mathbb{Z}_2)$, where 1 represents an identity operation. Let $M$ be a subgroup of a direct product of $E(3)$ and $\{1, 1'\}$. An element $(W, w)\theta$ of $M$
is called a magnetic symmetry operation, where $\theta \in \{1, 1'\}$ is a time-reversal part of the magnetic symmetry operation. In particular, $(W, w)1'$ is called an antisymmetry operation. A translation subgroup of $\mathcal{M}$ is defined similarly as

$$
\mathcal{T}(\mathcal{M}) := \{ (E, t) \mid \exists \theta \in \{1, 1'\}, (E, t)\theta \in \mathcal{M} \}.
$$

The subgroup $\mathcal{M}$ is called a magnetic space group (MSG) when its translation subgroup is generated from three independent translations. We write a magnetic point group of $\mathcal{M}$ as

$$
\mathcal{P}(\mathcal{M}) := \{ W\theta \mid \exists w \in \mathbb{R}^3, (W, w)\theta \in \mathcal{M} \}.
$$

We consider two derived space groups from $\mathcal{M}$. A family space group (FSG) of $\mathcal{M}$ is a space group obtained by ignoring time-reversal parts in magnetic symmetry operations:

$$
\mathcal{F}(\mathcal{M}) := \{ (W, w) \mid \exists \theta \in \{1, 1'\}, (W, w)\theta \in \mathcal{M} \}.
$$

A maximal space subgroup (XSG) of $\mathcal{M}$ is a space group obtained by removing antisymmetry operations:

$$
\mathcal{D}(\mathcal{M}) := \{ (W, w) \mid (W, w)1 \in \mathcal{M} \}.
$$

The MSGs are classified into the following four construct types (Bradley & Cracknell, 2009; Campbell et al., 2022):

- (Type I) $\mathcal{M} = \mathcal{F}(\mathcal{M})1 = \mathcal{D}(\mathcal{M})1$: The MSG $\mathcal{M}$ does not have antisymmetry operations.
- (Type II) $\mathcal{M} = \mathcal{F}(\mathcal{M})1 \sqcup \mathcal{F}(\mathcal{M})1', \mathcal{F}(\mathcal{M}) = \mathcal{D}(\mathcal{M})$: The MSG $\mathcal{M}$ has antisymmetry operations and corresponding ordinary symmetry operations.
- (Type III) $\mathcal{M} = \mathcal{D}(\mathcal{M})1 \sqcup (\mathcal{F}(\mathcal{M}) \setminus \mathcal{D}(\mathcal{M}))1'$ and $\mathcal{D}(\mathcal{M})$ is an index-two translationengleiche subgroup of $\mathcal{F}(\mathcal{M})$. Thus, translation subgroups of $\mathcal{F}(\mathcal{M})$ and $\mathcal{D}(\mathcal{M})$ are identical.
- (Type IV) $\mathcal{M} = \mathcal{D}(\mathcal{M}) \sqcup (\mathcal{F}(\mathcal{M}) \setminus \mathcal{D}(\mathcal{M}))$ and $\mathcal{D}(\mathcal{M})$ is an index-two kles-senleiche subgroup of $\mathcal{F}(\mathcal{M})$. Thus, point groups of $\mathcal{F}(\mathcal{M})$ and $\mathcal{D}(\mathcal{M})$ are identical.

For a type-III MSG example, Fig. 1(a) shows an antiferromagnetic (AFM) rutile structure whose MSG is $\mathcal{M}_{\text{rutile}} = \overline{P}4_12n'$ (BNS number 136.498) in magnetic Hall symbols (González-Platas et al., 2021). The FSG and XSG of $\mathcal{M}_{\text{rutile}}$ are $\overline{P}4_n2_n$ (No. 136) and $\overline{P}22_n$ (No. 58) in Hall symbols (Hall, 1981), respectively.

For a type-IV MSG example, Fig. 1(b) shows an AFM bcc structure whose MSG is $\mathcal{M}_{\text{bcc}} = \overline{P}4231'$ (BNS number 221.97) in magnetic Hall symbols. The FSG and XSG of $\mathcal{M}_{\text{bcc}}$ are $\overline{I}423$ (No. 229) and $\overline{P}423$ (No. 221) in Hall symbols, respectively.

### 2.2. Magnetic space-group type

We consider two coordinate systems specified with basis vectors $\mathbf{A} = (a_1, a_2, a_3)$ with origin $O$ and basis vectors $\mathbf{A}' = (a'_1, a'_2, a'_3)$ with origin $O'$. The other coordinate system is transformed to the another by a transformation $(\mathbf{P}, \mathbf{p})$ as

$$\mathbf{A}' = \mathbf{A} \mathbf{P}$$

$$\mathbf{A} \mathbf{p} = \mathbf{O}' - \mathbf{O},$$

where $\mathbf{P}$ is called the transformation matrix and $\mathbf{p}$ is called the origin shift. Point coordinates $\mathbf{x}$ are transformed by $(\mathbf{P}, \mathbf{p})$ to

$$\mathbf{x}' = (\mathbf{P}, \mathbf{p})^{-1} \mathbf{x} = \mathbf{P}^{-1}(\mathbf{x} - \mathbf{p}).$$

A symmetry operation $(\mathbf{W}, \mathbf{w})$ is transformed by $(\mathbf{P}, \mathbf{p})$ to

$$(\mathbf{W}', \mathbf{w}') = (\mathbf{P}, \mathbf{p})^{-1}(\mathbf{W}, \mathbf{w})(\mathbf{P}, \mathbf{p})$$

$$= (\mathbf{P}^{-1} \mathbf{W} \mathbf{P}, \mathbf{P}^{-1}(\mathbf{W} \mathbf{p} + \mathbf{w} - \mathbf{p})).$$

A transformation $(\mathbf{P}, \mathbf{p})$ with $\det \mathbf{P} > 0$ is orientation-preserving. When we regard two space groups as equivalent if they are transformed into each other by an orientation-
preserving transformation, each equivalent class of space groups is called a *space-group type*. We call a representative of each space-group type as the *space-group representative* and refer to the criteria for space groups to be chosen as a *setting*. The *standard ITA setting* is one of the conventional descriptions for each space-group type used in the *International Tables for Crystallography Vol. A* (Aroyo, 2016): unique axis b setting, cell choice 1 for monoclinic groups, hexagonal axes for rhombohedral groups, and origin choice 2 for centrosymmetric groups.

We assume that a magnetic symmetry operation \((W, w)\theta\) is transformed by \((P, p)\) as

\[
(W', w') = (P, p)^{-1}(W, w)(P, p)
\]

\[
\theta' = \theta.
\]

Similarly to space groups, each equivalent class of MSGs up to orientation-preserving transformations is called a *magnetic space-group type*.

### 2.3. BNS setting

The BNS symbol represents each magnetic space-group type (Belov *et al.*, 1957). We refer to a setting of the BNS symbol as a *BNS setting*: For types-I, -II, and -III MSGs, it uses the same setting as the standard ITA setting of the FSG. For type-IV MSG, it uses that of the XSG. In Sec. 4, we standardize a given magnetic crystal structure by applying a transformation to an MSG in the BNS setting.

### 2.4. Action of magnetic symmetry operations

In general, we can arbitrarily choose how magnetic symmetry operation acts on objects as long as it satisfies the definition of left actions. Here, we show examples of actions on collinear and non-collinear magnetic moments.

For a collinear magnetic moment \(m\) without spin–orbit coupling, magnetic symme-
try operations act on it as follows:

\[(W, w)m = m\]  
\[(14)\]

\[1'm = -m.\]  
\[(15)\]

For a non-collinear magnetic moment \(m\), magnetic symmetry operations act on it as follows:

\[(W, w)m = (\det W)AWA^{-1}m\]  
\[(16)\]

\[1'm = -m,\]  
\[(17)\]

where we choose the Cartesian coordinate to represent \(m\).

### 3. Magnetic symmetry operation search

A magnetic crystal structure is represented by the following four objects: (1) basis vectors of its lattice \(A = (a_1, a_2, a_3)\), (2) an array of point coordinates of sites in its unit cell \(X = (x_1, \cdots, x_N)\), (3) an array of atomic types of sites in its unit cell \(T = (t_1, \cdots, t_N)\), and (4) an array of magnetic moments of sites in its unit cell \(M = (m_1, \cdots, m_N)\), where \(N\) is the number of sites in the unit cell. We formulate an MSG of the magnetic crystal structure \((A, X, T, M)\) as a stabilizer subgroup of \(E(3)\). Then, we provide an algorithm for determining the magnetic symmetry operations on the basis of equivalence relationships between sites in the magnetic crystal structure. A schematic diagram of the MSG and related space groups is shown in Fig. 2.

First, we consider a crystal structure \((A, X, T)\) obtained by ignoring magnetic moments of \((A, X, T, M)\). A space group of \((A, X, T)\) is written as a stabilizer subgroup of \(E(3)\) that preserves \((A, X, T, M)\):

\[S(A, X, T) := \text{Stab}_{E(3)} (A, X, T)\]

\[= \left\{ g \in E(3) \mid \begin{array}{l} \exists \sigma_g \in \mathcal{S}_N, \forall i, \\
gx_i \equiv x_{\sigma_g(i)} \pmod{1} \\
l_i = l_{\sigma_g(i)} \end{array} \right\},\]  
\[(18)\]

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An MSG of \((A, X, T, M)\) is similarly written as a stabilizer subgroup of \(E(3) \times \{1, 1'\}\) that preserves \((A, X, T, M)\):

\[
\mathcal{M}(A, X, T, M) := \text{Stab}_{E(3) \times \{1, 1'\}}(A, X, T, M)
\]

\[
= \left\{ g\theta \in E(3) \times \{1, 1'\} \mid \exists \sigma_g \in \mathfrak{S}_N, \forall i, \\
gx_i \equiv x_{\sigma_g(i)} \pmod{1} \\
t_i = t_{\sigma_g(i)}, \\
g\theta m_i = m_{\sigma_g(i)} \right\}.
\]  

\[\text{(19)}\]

In the last line of the above equations, we can confine the domain of symmetry operations \(g\) to \(S(A, X, T)\) because time-reversal operations do not change point coordinates and atomic types.

Equation (19) also gives a procedure to search for magnetic symmetry operations. First, we compute \(S(A, X, T)\) and a permutation \(\sigma_g\) for each symmetry operation \(g \in S(A, X, T)\). Then, we check if magnetic moments satisfy \(g\theta m_i = m_{\sigma_g(i)}\) for \(\theta = 1\) and \(\theta = 1'\). Note that magnetic symmetry operations \(g\theta\) with both \(\theta = 1\) and \(\theta = 1'\) may belong to \(\mathcal{M}(A, X, T, M)\) when all magnetic moments are zero (in this case, the MSG is type II).

The FSG and XSG of \((A, X, T, M)\) are written with \(\mathcal{M}(A, X, T, M)\) as

\[
\mathcal{F}(A, X, T, M) := \mathcal{F}(\mathcal{M}(A, X, T, M))
\]

\[
= \left\{ g \mid \exists \theta \in \{1, 1'\}, \\
g\theta \in \mathcal{M}(A, X, T, M) \right\}
\]  

\[\text{(20)}\]

\[
\mathcal{D}(A, X, T, M) := \mathcal{D}(\mathcal{M}(A, X, T, M))
\]

\[
= \{ g \mid g1 \in \mathcal{M}(A, X, T, M) \}.
\]  

\[\text{(21)}\]
because the former ignores magnetic moments.

Note that the comparison of point coordinates and magnetic moments should be performed within tolerances in practice (Grosse-Kunstleve et al., 2004). We use an absolute tolerance parameter $\epsilon$ for point coordinates (Togo & Tanaka, 2018) and another absolute tolerance $\epsilon_{\text{mag}}$ for magnetic moments. Then, the comparisons in this section are replaced with the following inequalities:

$$\begin{align*}
gx_i = x_{\sigma_g(i)} \mod 1 \Rightarrow \left\| A \left[ gx_i - x_{\sigma_g(i)} \right] \mod 1 \right\|_2 < \epsilon \\
g\theta m_i = m_{\sigma_g(i)} \Rightarrow \left\| g\theta m_i - m_{\sigma_g(i)} \right\|_2 < \epsilon_{\text{mag}}.
\end{align*}$$

(22) \hspace{2cm} (23)

Here, $[\cdot]_{\mod 1}$ takes a remainder with modulo one between $[-0.5, 0.5]$. 

### 4. Identification of magnetic space-group type

We identify a magnetic space-group type for the determined MSG $\mathcal{M} := \mathcal{M}(A, X, T, M)$. For all the 1651 magnetic space-group types, a magnetic space-group representative $\mathcal{M}_{\text{std}}$ in the BNS setting has already been tabulated (González-Platas et al., 2021; Campbell et al., 2022). Thus, we search for $\mathcal{M}_{\text{std}}$ with the same magnetic space-group type as $\mathcal{M}$ and an orientation-preserving transformation $(P, p)$ while satisfying

$$(P, p)^{-1} \mathcal{M}(P, p) = \mathcal{M}_{\text{std}}.$$  

(24)

In Sec. 4.1 we identify a construct type of $\mathcal{M}$ to choose a candidate $\mathcal{M}_{\text{std}}$, which is one of the magnetic space-group representatives in the BNS setting. In Sec. 4.2 we try to obtain $(P, p)$ from affine normalizers of $\mathcal{F}(\mathcal{M}_{\text{std}})$ or $\mathcal{D}(\mathcal{M}_{\text{std}})$.

#### 4.1. Identification of construct type of MSG

The construct type of $\mathcal{M}$ can be determined from orders of the magnetic point group and point groups of FSG and XSG. When $|\mathcal{P}(\mathcal{F}(\mathcal{M}))|/|\mathcal{P}(\mathcal{D}(\mathcal{M}))| = 1$, $\mathcal{M}$ is type I or
II. Then, when $|\mathcal{P}(\mathcal{M})|/|\mathcal{P}(\mathcal{F}(\mathcal{M}))| = 1$, $\mathcal{M}$ is type I. When $|\mathcal{P}(\mathcal{M})|/|\mathcal{P}(\mathcal{F}(\mathcal{M}))| = 2$, $\mathcal{M}$ is type II.

When $|\mathcal{P}(\mathcal{F}(\mathcal{M}))|/|\mathcal{P}(\mathcal{D}(\mathcal{M}))| = 2$, $\mathcal{M}$ is type III or IV. For type-III or type-IV MSG, we consider a coset decomposition of $\mathcal{M}$ by $\mathcal{D}(\mathcal{M})$:

$$\mathcal{M} = \mathcal{D}(\mathcal{M})1 \sqcup \mathcal{D}(\mathcal{M})(\mathbf{w}_0,\mathbf{w}_0)1'.$$

(25)

If the coset representative $(\mathbf{w}_0,\mathbf{w}_0)1'$ can be taken as an anti-translation, $\mathcal{D}(\mathcal{M})$ is a klessengleiche subgroup of $\mathcal{F}(\mathcal{M})$ and $\mathcal{M}$ is type IV. If not, $\mathcal{D}(\mathcal{M})$ is a translationengleiche subgroup of $\mathcal{F}(\mathcal{M})$ and $\mathcal{M}$ is type III.

4.2. Comparison with MSGs in BNS setting

As shown in Appendix A, the condition in Eq. (24) is equivalent to satisfying the following two conditions:

$$(\mathbf{P}p)^{-1}\mathcal{F}(\mathcal{M})(\mathbf{P}p) = \mathcal{F}(\mathcal{M}_{\text{std}})$$

(26)

$$(\mathbf{P}p)^{-1}\mathcal{D}(\mathcal{M})(\mathbf{P}p) = \mathcal{D}(\mathcal{M}_{\text{std}}).$$

(27)

Since $\mathcal{M}_{\text{std}}$ is a magnetic space-group representative in the BNS setting, we divide the identification procedure by cases when $\mathcal{M}$ is type IV or otherwise.

4.2.1. When $\mathcal{M}$ is type I, II, or III When $\mathcal{M}$ is type I, II, or III, we obtain an orientation-preserving transformation $(\mathbf{P}',\mathbf{p}')$ between $\mathcal{F}(\mathcal{M})$ and $\mathcal{F}(\mathcal{M}_{\text{std}})$, where $\mathcal{M}_{\text{std}}$ has the same contract type as $\mathcal{M}$ and $\mathcal{F}(\mathcal{M}_{\text{std}})$ has the same space-group type as $\mathcal{F}(\mathcal{M})$. An algorithm to obtain $(\mathbf{P}',\mathbf{p}')$ has been given by Grosse-Kunstleve (1999) and Togo & Tanaka (2018). We write an MSG transformed by $(\mathbf{P}',\mathbf{p}')$ as

$$\mathcal{M}' := (\mathbf{P}',\mathbf{p}')^{-1}\mathcal{M}(\mathbf{P}',\mathbf{p}').$$

(28)

By construction, $\mathcal{F}(\mathcal{M}')$ and $\mathcal{F}(\mathcal{M}_{\text{std}})$ are identical. Also, $\mathcal{F}(\mathcal{M}')$ is the space-group representative in the standard ITA setting.
Note that such an orientation-preserving transformation \((P', p')\) is not unique: in general, orientation-preserving transformations in an affine normalizer of \(F(M_{\text{std}})\) give the identical conjugated space group (Koch et al., 2016). We write the affine normalizer of a space group \(S\) as

\[
\mathcal{N}_{A(3)}(S) := \{(Q, q) \in A(3) \mid (Q, q)^{-1}S(Q, q) = S\},
\]

where \(A(3)\) is the three-dimensional affine group.

When \(M\) is type I or II, the XSGs are also identical, \(D(M') = F(M') = F(M_{\text{std}}) = D(M_{\text{std}})\). Thus, \((P', p')\) also satisfies Eq. (24). However, when \(M\) is type III, we additionally need to search for an orientation-preserving transformation \((P_{\text{corr}}, p_{\text{corr}})\) \(\in \mathcal{N}_{A(3)}(F(M_{\text{std}}))\) such that

\[
(P_{\text{corr}}, p_{\text{corr}})^{-1}D(M')(P_{\text{corr}}, p_{\text{corr}}) = D(M_{\text{std}}).
\]

(30)

The situation is shown in Fig. 3(a).

When \(F(M_{\text{std}})\) is triclinic or monoclinic, there are no such conjugate space groups with \(D(M') \neq D(M_{\text{std}})\) because \(P(F(M_{\text{std}}))\) does not have a pair of proper conjugate subgroups. For other cases, we need to compute \(\mathcal{N}_{A(3)}(F(M_{\text{std}}))\) and search for \((P_{\text{corr}}, p_{\text{corr}})\) that satisfies Eq. (30). Instead of computing or tabulating \(\mathcal{N}_{A(3)}(F(M_{\text{std}}))\), we enumerate linear parts and origin shifts of orientation-preserving transformations in \(\mathcal{N}_{A(3)}(F(M_{\text{std}}))\) as follows. For linear parts, we enumerate integer matrices \(P_{\text{corr}}\) whose elements are -1, 0, or 1, and their determinant are equal to one. For origin shifts, we enumerate vectors \(p_{\text{corr}}\) by restricting their values to one of \(\{0, \frac{1}{4}, \frac{1}{3}, \frac{1}{2}, \frac{2}{3}, \frac{3}{4}\}\). These will be sufficient because they cover all orientation-preserving coset representatives of \(\mathcal{N}_{A(3)}(F(M_{\text{std}}))/F(M_{\text{std}})\) up to translations (Koch et al., 2016). Since \((P_{\text{corr}}, p_{\text{corr}})\) can be tabulated for each space-group representative in the standard ITA setting, we can precompute and reuse them. If one of the precomputed transformations satisfies
Eq. (30), a combined transformation

\[
(P, p) := (P', p')(P_{\text{corr}}, p_{\text{corr}})
\]  

(31)

holds Eq. (24) and transforms \( \mathcal{M} \) to \( \mathcal{M}_{\text{std}} \).

4.2.2. When \( \mathcal{M} \) is type IV

When \( \mathcal{M} \) is type IV, we obtain an orientation-preserving transformation \((P', p')\) between \( \mathcal{D}(\mathcal{M}) \) and \( \mathcal{D}(\mathcal{M}_{\text{std}}) \), where \( \mathcal{M}_{\text{std}} \) has the same contract type as \( \mathcal{M} \) and \( \mathcal{D}(\mathcal{M}_{\text{std}}) \) has the same space-group type as \( \mathcal{D}(\mathcal{M}) \). Then, the XSG of the transformed MSG in Eq. (28), \( \mathcal{D}(M') \), is the space-group representative in the standard ITA setting.

Similarly to type-III MSGs, we need to search for an orientation-preserving transformation \((P_{\text{corr}}, p_{\text{corr}}) \in \mathcal{N}_A(3)(\mathcal{D}(\mathcal{M}_{\text{std}}))\) such that

\[
(P_{\text{corr}}, p_{\text{corr}})^{-1} \mathcal{F}(M')(P_{\text{corr}}, p_{\text{corr}}) = \mathcal{F}(M_{\text{std}}).
\]  

(32)

The situation is shown in Fig. 3(b).

When \( \mathcal{D}(\mathcal{M}_{\text{std}}) \) is neither triclinic nor monoclinic, the brute-force tabulation in Sec. 4.2.1 also works for \( \mathcal{N}_A(3)(\mathcal{D}(\mathcal{M}_{\text{std}})) \). For triclinic and monoclinic cases, a factor group \( \mathcal{N}_A(3)(\mathcal{D}(\mathcal{M}_{\text{std}}))/\mathcal{D}(\mathcal{M}_{\text{std}}) \) is not finite, and we cannot prove the completeness in the same manner. Thus, we show that the enumerated \((P_{\text{corr}}, p_{\text{corr}})\) covers all conjugated type-IV MSGs by explicitly listing \((P_{\text{corr}}, p_{\text{corr}})\) and the conjugated MSGs in Appendix B.

4.2.3. Examples of conjugated MSGs

We present examples of conjugated MSGs for type III and type IV. For a type-III MSG example, consider coset representatives of

\footnote{The FSG \( \mathcal{F}(M_{\text{std}}) \) is a subgroup of \( \mathcal{N}_A(3)(\mathcal{D}(\mathcal{M}_{\text{std}})) \): because \( \mathcal{D}(\mathcal{M}_{\text{std}}) \) is a normal subgroup of \( \mathcal{F}(\mathcal{M}_{\text{std}}) \), every operation in \( \mathcal{F}(\mathcal{M}_{\text{std}}) \) stabilizes \( \mathcal{D}(\mathcal{M}_{\text{std}}) \) and belongs to \( \mathcal{N}_A(3)(\mathcal{D}(\mathcal{M}_{\text{std}})) \). Similarly, \( \mathcal{F}(M') \) is a subgroup of \( \mathcal{N}_A(3)(\mathcal{D}(\mathcal{M}_{\text{std}})) \).}
\( M_{\text{std}} \) in the BNS setting (BNS number 17.10) as follows:

\[
\begin{align*}
&x, y, z, 1; x, -y, -z, 1; \\
&- x, -y, z + 1/2, 1'; -x, y, -z + 1/2, 1'.
\end{align*}
\]

There is another MSG \( M' \) with the same magnetic space-group type as \( M_{\text{std}} \) and identical FSG to \( M_{\text{std}} \):

\[
\begin{align*}
&x, y, z, 1; -x, y, -z + 1/2, 1; \\
&- x, -y, z + 1/2, 1'; x, -y, -z, 1'.
\end{align*}
\]

Although \( D(M_{\text{std}}) \) and \( D(M') \) belong to the same space-group type (No. 3), these XSGs are different. The following transformation maps \( M' \) to \( M_{\text{std}} \) while satisfying Eq. (30):

\[
(P_{\text{corr}}, p_{\text{corr}}) = \begin{pmatrix}
0 & -1 & 0 \\
-1 & 0 & 0 \\
0 & 0 & -1
\end{pmatrix}, \begin{pmatrix}
0 \\
0 \\
\frac{1}{2}
\end{pmatrix}.
\]

For a type-IV MSG example, consider coset representatives of \( M_{\text{std}} \) in the BNS setting (BNS number 9.40) as follows:

\[
\begin{align*}
&x, y, z, 1; x, -y, z + 1/2, 1; \\
&x + 1/2, y + 1/2, z, 1; x + 1/2, -y + 1/2, z + 1/2, 1; \\
&x + 1/2, -y + 1/2, z, 1'; x, -y, z, 1'; \\
&x, y, z + 1/2, 1'; x + 1/2, y + 1/2, z + 1/2, 1'.
\end{align*}
\]

There is another MSG \( M' \) with the same magnetic space-group type as \( M_{\text{std}} \) and identical XSG to \( M_{\text{std}} \):

\[
\begin{align*}
&x, y, z, 1; x + 1/2, -y + 1/2, z + 1/2, 1; \\
&x + 1/2, y + 1/2, z, 1; x, -y, z + 1/2, 1; \\
&x + 1/2, -y, z, 1'; x, -y + 1/2, z, 1'; \\
&x + 1/2, y, z + 1/2, 1'; x, y + 1/2, z + 1/2, 1'.
\end{align*}
\]
Although $\mathcal{F}(\mathcal{M}_{\text{std}})$ and $\mathcal{F}(\mathcal{M}')$ belong to the same space-group type (No. 8), these FSGs are different. The following transformation maps $\mathcal{M}'$ to $\mathcal{M}_{\text{std}}$ while satisfying Eq. (32):

\[
(P_{\text{corr}}, p_{\text{corr}}) = \left( \begin{pmatrix} -1 & 0 & -1 \\ 0 & -1 & 0 \\ 0 & 0 & 1 \end{pmatrix}, \begin{pmatrix} 0 \\ 1/3 \\ 0 \end{pmatrix} \right).
\]

5. Symmetrization of magnetic crystal structure

We symmetrize the magnetic crystal structure $(A, X, T, M)$ by magnetic symmetry operations of the determined MSG $\mathcal{M}(A, X, T, M)$. For convenience, we consider its coset decomposition with a finite index as follows. Let $\mathcal{T}_A$ be a translation group formed by basis vectors $A$, which may not be primitive basis vectors. We write a coset decomposition of $\mathcal{M}(A, X, T, M)$ by $\mathcal{T}_A$ as

\[
\mathcal{M}(A, X, T, M) = \bigsqcup_{\kappa} (W_\kappa, w_\kappa) \theta_\kappa \mathcal{T}_A. \tag{33}
\]

We write the set of coset representatives as

\[
\overline{\mathcal{M}} := \{(W_\kappa, w_\kappa) \theta_\kappa\}_\kappa. \tag{34}
\]

A centering operation $(E, w)1$, where $w \not\equiv 0 \ (\mod 1)$, may belong to $\overline{\mathcal{M}}$.

A procedure to symmetrize the array of point coordinates $X$ by $\overline{\mathcal{M}}$ is essentially the same as those used by Grosse-Kunstleve & Adams (2002) and Togo & Tanaka (2018). For the $\kappa$th magnetic symmetry operation $(W_\kappa, w_\kappa) \theta_\kappa$, we denote that its inverse maps the $\sigma_\kappa^{-1}(i)$th point coordinates to the $i$th point coordinates. Then, $(W_\kappa, w_\kappa)x_{\sigma_\kappa^{-1}(i)}$ should be close to $x_i$ up to lattice translations in $\mathcal{T}_A$. With this observation, each of the point coordinates $x_i$ can be symmetrized to $\tilde{x}_i$ by a projection operator:

\[
\tilde{x}_i := x_i + \frac{1}{|\overline{\mathcal{M}}|} \sum_{\kappa} \left[ (W_\kappa, w_\kappa)x_{\sigma_\kappa^{-1}(i)} - x_i \right]_{\mod 1}. \tag{35}
\]
The modulo is required because the original and mapped point coordinates in the unit cell may be displaced by lattice translations.

A procedure to symmetrize the array of magnetic moments $M$ is similar to that to symmetrize the array of point coordinates. Each magnetic moment $m_i$ can be symmetrized to $\tilde{m}_i$ by the following projection operator:

$$\tilde{m}_i := \frac{1}{|M|} \sum_{\kappa} (W_{\kappa}, w_{\kappa}) \theta_{\kappa} m_{\kappa^{-1}(i)}. \quad (36)$$

6. Conclusion

We have presented the algorithms for determining magnetic symmetry operations for a given magnetic crystal structure, identifying a magnetic space-group type for a given MSG, and symmetrizing the magnetic crystal structure on the basis of the determined MSG. Linear and translation parts of magnetic symmetry operations are determined from the crystal structure by ignoring magnetic moments. A transformation between the determined MSG and a BNS-setting MSG is obtained by considering affine normalizers: that of the FSG for type-I, -II, or -III MSGs and that of the XSG for type-IV MSGs. In particular, we provide exhaustive tables of conjugated MSGs with triclinic or monoclinic type-IV MSGs in the BNS setting and corresponding transformations. Projection operators of the determined MSG symmetrize point coordinates and magnetic moments of the magnetic crystal structure. These algorithms are designed comprehensively and implemented in SPGLIB under the BSD 3-clause license. The present algorithms and their implementations are expected to contribute to computational crystallography and materials science, including high-throughput first-principles calculations and crystal structure predictions.

Appendix A
Condition that two MSGs are identical

For two MSGs $\mathcal{M}_1$ and $\mathcal{M}_2$, we write the FSG and XSG of $\mathcal{M}_i (i = 1, 2)$ as $\mathcal{F}_i$ and $\mathcal{D}_i$, respectively. When $\mathcal{M}_1$ and $\mathcal{M}_2$ have the same construct types, they are identical if and only if their FSGs and XSGs are also identical, that is, $\mathcal{F}_1 = \mathcal{F}_2$ and $\mathcal{D}_1 = \mathcal{D}_2$. Although it is trivial, we give proof of this fact for completeness.

When $\mathcal{M}_1$ and $\mathcal{M}_2$ are identical, their FSGs and XSGs are also identical by definition. We check the converse for each construct type. For type-I MSGs, $\mathcal{M}_1 = \mathcal{F}_1 \mathcal{F}_1' = \mathcal{F}_2 \mathcal{F}_2' = \mathcal{M}_2$. For type-II MSGs, $\mathcal{M}_1 = \mathcal{F}_1 \mathcal{F}_1' \mathcal{F}_1 = \mathcal{F}_2 \mathcal{F}_2' \mathcal{F}_2 = \mathcal{M}_2$. For type-III or type-IV MSGs, $\mathcal{M}_1 = \mathcal{D}_1 \mathcal{D}_1' \mathcal{F}_1 \mathcal{D}_1' = \mathcal{D}_2 \mathcal{D}_2' \mathcal{F}_2 \mathcal{D}_2' = \mathcal{M}_2$. Thus, if FSGs and XSGs are identical, the two MSGs are also identical.

Appendix B
Correction transformations for triclinic or monoclinic type-IV MSGs

We give all anti-translations in conjugated MSGs and corresponding transformations $(P, p)$ for a type-IV MSG $\mathcal{M}_{\text{std}}$ in the BNS setting, where $\mathcal{D}(\mathcal{M}_{\text{std}})$ is triclinic or monoclinic. Because an anti-translation $(E, w)l'$ in a type-IV MSG is index-two up
to translations, it is sufficient to consider the following seven anti-translations:

\[ 1'_a = \left( E, \left( \frac{1}{2}, 0, 0 \right) \right) 1' \quad (37) \]
\[ 1'_b = \left( E, \left( 0, \frac{1}{2}, 0 \right) \right) 1' \quad (38) \]
\[ 1'_c = \left( E, \left( 0, 0, \frac{1}{2} \right) \right) 1' \quad (39) \]
\[ 1'_bc = \left( E, \left( 0, \frac{1}{2}, \frac{1}{2} \right) \right) 1' \quad (40) \]
\[ 1'_ac = \left( E, \left( \frac{1}{2}, 0, \frac{1}{2} \right) \right) 1' \quad (41) \]
\[ 1'_ab = \left( E, \left( \frac{1}{2}, \frac{1}{2}, 0 \right) \right) 1' \quad (42) \]
\[ 1'_{abc} = \left( E, \left( \frac{1}{2}, \frac{1}{2}, \frac{1}{2} \right) \right) 1'. \quad (43) \]

When \( \mathcal{D}(\mathcal{M}_{\text{std}}) \) is a triclinic or monoclinic P-centering space group (Nos. 1, 2, 3, 4, 6, 7, 10, 11, 13, and 14), Tables 1, 2, 3, 4, 6, 7, 10, 11, 13, and 14 show transformations for \( \mathcal{M}_{\text{std}} \), which are obtained by the brute force described in Sec. 4.2.1 and anti-translations in the transformed MSGs. Because each table contains the seven anti-translations, we confirm that these transformations are sufficient to search for conjugated type-IV MSGs.

For other cases, \( \mathcal{D}(\mathcal{M}_{\text{std}}) \) is a monoclinic C-centering space group (Nos. 5, 8, 9, 12, and 15). Tables 5, 8, 9, 12, and 15 show transformations for \( \mathcal{M}_{\text{std}} \) and anti-translations in the transformed MSGs. Note that the anti-translation \( 1'_{ab} \) should not be contained in the conjugated MSGs because \( \mathcal{M}_{\text{std}} \) is not type II and \( \mathcal{D}(\mathcal{M}_{\text{std}}) \) is C-centering. Then, each table contains the six anti-translations other than \( 1'_{ab} \). Thus, we also confirm that these transformations are sufficient.

We would like to thank Juan Rodríguez-Carvajal for providing magnetic space-group datasets.

This work was supported by a Grant-in-Aid for JSPS Research Fellows (Grant Number 21J10712) from the Japan Society for the Promotion of Science (JSPS).
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Fig. 1. Examples of antiferromagnetic (AFM) crystal structures with (a) type-III and (b) type-IV MSGs. The red arrows represent collinear spins with the same magnitudes.

Fig. 2. Group–subgroup relationship of MSGs and related space groups. The nodes represent space groups or MSGs. Each edge indicates that a lower group is a subgroup of an upper group in the diagram.
Fig. 3. Group–subgroup relationship of conjugated MSGs and affine normalizers.

Table 1. Transformations between type-IV MSG \( \mathcal{M}_{\text{std}} \) and conjugated MSGs, where their XSGs are identical to a space group of No. 1 in the ITA standard setting.

| BNS number | Transformation \((P, p)\) | Anti-translations in \((P, p)^{-1} \mathcal{M}_{\text{std}}(P, p)\) |
|------------|-----------------|------------------|
| 1.3        | \((E, 0)\)       | \(1'_{bc}\)       |
|            | \[\begin{pmatrix} 0 & -1 & -1 \\ 0 & -1 & 0 \\ -1 & -1 & -1 \end{pmatrix}, 0\] | \(1'_{ac}\)       |
|            | \[\begin{pmatrix} -1 & 0 & -1 \\ -1 & 0 & -1 \\ -1 & -1 & -1 \end{pmatrix}, 0\] | \(1'_{abc}\)      |
|            | \[\begin{pmatrix} -1 & 0 & -1 \\ 0 & -1 & -1 \\ -1 & -1 & -1 \end{pmatrix}, 0\] | \(1'_{ab}\)       |
|            | \[\begin{pmatrix} -1 & 0 & -1 \\ -1 & -1 & 0 \\ -1 & 0 & -1 \end{pmatrix}, 0\] | \(1'_{ac}\)       |
|            | \[\begin{pmatrix} -1 & 0 & -1 \\ -1 & 0 & -1 \\ -1 & 0 & -1 \end{pmatrix}, 0\] | \(1'_{bc}\)       |
|            | \[\begin{pmatrix} 0 & -1 & -1 \\ -1 & 0 & -1 \\ -1 & -1 & -1 \end{pmatrix}, 0\] | \(1'_{b}\)        |
|            | \[\begin{pmatrix} -1 & 0 & -1 \\ -1 & 0 & -1 \\ -1 & -1 & -1 \end{pmatrix}, 0\] | \(1'_{a}\)        |
|            | \[\begin{pmatrix} 0 & -1 & -1 \\ -1 & -1 & -1 \\ -1 & -1 & 0 \end{pmatrix}, 0\] | \(1'_{c}\)        |
### Table 2. Transformations between type-IV MSG $\mathcal{M}_{\text{std}}$ and conjugated MSGs, where their XSGs are identical to a space group of No. 2 in the ITA standard setting.

| BNS number | Transformation $(P, p)$ | $\mathcal{M}_{\text{std}}^{-1}$ | Anti-translations in $(P, p)^{-1} \mathcal{M}_{\text{std}}(P, p)$ |
|------------|-------------------------|---------------------------------|---------------------------------------------------------------|
| 2.7        | $(E, 0)$                |                                 | $I_c'$                                                         |
|            | $\begin{pmatrix} 0 & -1 & -1 \\ 0 & -1 & 0 \\ -1 & -1 & -1 \end{pmatrix}$ | $1_a'$                                      |                                                               |
|            | $\begin{pmatrix} -1 & 0 & -1 \\ -1 & 0 & 0 \\ -1 & 1 & -1 \end{pmatrix}$ | $1_b'$                                      |                                                               |
|            | $\begin{pmatrix} -1 & -1 & -1 \\ -1 & 0 & 0 \\ -1 & -1 & -1 \end{pmatrix}$ | $1_{bc}$                                     |                                                               |
|            | $\begin{pmatrix} -1 & 0 & -1 \\ -1 & -1 & -1 \\ -1 & 0 & 0 \end{pmatrix}$ | $1_{ac}$                                     |                                                               |
|            | $\begin{pmatrix} 0 & -1 & -1 \\ -1 & -1 & -1 \\ -1 & 0 & 0 \end{pmatrix}$ | $1_{ab}$                                     |                                                               |
|            | $\begin{pmatrix} -1 & -1 & 0 \\ -1 & -1 & 0 \\ -1 & 0 & 0 \end{pmatrix}$ | $1_{abc}$                                    |                                                               |

### Table 3. Transformations between type-IV MSG $\mathcal{M}_{\text{std}}$ and conjugated MSGs, where their XSGs are identical to a space group of No. 3 in the ITA standard setting.

| BNS number | Transformation $(P, p)$ | $\mathcal{M}_{\text{std}}^{-1}$ | Anti-translations in $(P, p)^{-1} \mathcal{M}_{\text{std}}(P, p)$ |
|------------|-------------------------|---------------------------------|---------------------------------------------------------------|
| 3.4        | $(E, 0)$                |                                 | $1_a'$                                                         |
|            | $\begin{pmatrix} -1 & 0 & -1 \\ 0 & -1 & 0 \\ -1 & 0 & 0 \end{pmatrix}$ | $1_c'$                                      |                                                               |
|            | $\begin{pmatrix} -1 & 0 & 0 \\ 0 & -1 & 0 \\ -1 & 0 & 1 \end{pmatrix}$ | $1_{ac}$                                     |                                                               |
| 3.5        | $(E, 0)$                |                                 | $1_b'$                                                         |
| 3.6        | $(E, 0)$                |                                 | $1_{ab}$                                                       | $1_{bc}$                                                       |
|            | $\begin{pmatrix} -1 & 0 & -1 \\ 0 & -1 & 0 \\ -1 & 0 & 0 \end{pmatrix}$ | $1_{bc}$                                     |                                                               |
|            | $\begin{pmatrix} -1 & 0 & 0 \\ 0 & -1 & 0 \\ -1 & 0 & 1 \end{pmatrix}$ | $1_{abc}$                                    |                                                               |
Table 4. Transformations between type-IV MSG $M_{\text{std}}$ and conjugated MSGs, where their XSGs are identical to a space group of No. 4 in the ITA standard setting.

| BNS number | Transformation $(P, p)$ | Anti-translations in $(P, p)^{-1}M_{\text{std}}(P, p)$ |
|------------|-------------------------|-----------------------------------------------------|
| 4.10       | $(E, 0)$                | $1'_{a}$                                           |
|            | $(-1 0 -1)$             |                                                     |
|            | $0 -1 0$                |                                                     |
|            | $(-1 0 0)$              |                                                     |
|            | $0 -1 0$                |                                                     |
|            | $(-1 0 1)$              |                                                     |
| 4.11       | $(E, 0)$                | $1'_{b}$                                           |
| 4.12       | $(E, 0)$                | $1'_{ab}$                                          |

Table 5. Transformations between type-IV MSG $M_{\text{std}}$ and conjugated MSGs, where their XSGs are identical to a space group of No. 5 in the ITA standard setting.

| BNS number | Transformation $(P, p)$ | Anti-translations in $(P, p)^{-1}M_{\text{std}}(P, p)$ |
|------------|-------------------------|-----------------------------------------------------|
| 5.16       | $(E, 0)$                | $1'_{c}, 1'_{abc}$                                   |
|            | $(-1 0 -1)$             |                                                     |
|            | $0 -1 0$                |                                                     |
|            | $(-1 0 0)$              |                                                     |
|            | $0 -1 0$                |                                                     |
|            | $(-1 0 1)$              |                                                     |
| 5.17       | $(E, 0)$                | $1'_{a}, 1'_{b}$                                     |

Table 6. Transformations between type-IV MSG $M_{\text{std}}$ and conjugated MSGs, where their XSGs are identical to a space group of No. 6 in the ITA standard setting.

| BNS number | Transformation $(P, p)$ | Anti-translations in $(P, p)^{-1}M_{\text{std}}(P, p)$ |
|------------|-------------------------|-----------------------------------------------------|
| 6.21       | $(E, 0)$                | $1'_{a}$                                           |
|            | $(-1 0 -1)$             |                                                     |
|            | $0 -1 0$                |                                                     |
|            | $(-1 0 0)$              |                                                     |
|            | $0 -1 0$                |                                                     |
|            | $(-1 0 1)$              |                                                     |
| 6.22       | $(E, 0)$                | $1'_{b}$                                           |
| 6.23       | $(E, 0)$                | $1'_{ab}$                                          |
|            | $(-1 0 -1)$             |                                                     |
|            | $0 -1 0$                |                                                     |
|            | $(-1 0 0)$              |                                                     |
|            | $0 -1 0$                |                                                     |
|            | $(-1 0 1)$              |                                                     |
Table 7. Transformations between type-IV MSG $\mathcal{M}_{\text{std}}$ and conjugated MSGs, where their XSGs are identical to a space group of No. 7 in the ITA standard setting.

| BNS number | Transformation $(P, p)$ | Anti-translations in $(P, p)^{-1}\mathcal{M}_{\text{std}}(P, p)$ |
|------------|------------------------|---------------------------------------------------------------|
| 7.27       | $(E, 0)$                | $\begin{pmatrix} 1_a \end{pmatrix}$                         |
|            | $\begin{pmatrix} -1 & 0 & 0 \\ 0 & -1 & 0 \\ -1 & 0 & 1 \end{pmatrix}, 0$ | $\begin{pmatrix} 1'_a \end{pmatrix}$                         |
| 7.28       | $(E, 0)$                | $\begin{pmatrix} 1'_{bc} \end{pmatrix}$                      |
| 7.29       | $(E, 0)$                | $\begin{pmatrix} 1'_b \end{pmatrix}$                         |
| 7.30       | $(E, 0)$                | $\begin{pmatrix} 1'_{ab} \end{pmatrix}$                      |
|            | $\begin{pmatrix} -1 & 0 & 0 \\ 0 & -1 & 0 \\ -1 & 0 & 1 \end{pmatrix}, 0$ | $\begin{pmatrix} 1'_{abc} \end{pmatrix}$                      |
| 7.31       | $(E, 0)$                | $\begin{pmatrix} 1'_c \end{pmatrix}$                         |

Table 8. Transformations between type-IV MSG $\mathcal{M}_{\text{std}}$ and conjugated MSGs, where their XSGs are identical to a space group of No. 8 in the ITA standard setting.

| BNS number | Transformation $(P, p)$ | Anti-translations in $(P, p)^{-1}\mathcal{M}_{\text{std}}(P, p)$ |
|------------|------------------------|---------------------------------------------------------------|
| 8.35       | $(E, 0)$                | $\begin{pmatrix} 1'_{c}, 1'_{abc} \end{pmatrix}$            |
|            | $\begin{pmatrix} -1 & 0 & -1 \\ 0 & -1 & 0 \\ 0 & 0 & 1 \end{pmatrix}, 0$ | $\begin{pmatrix} 1'_{ac}, 1'_{bc} \end{pmatrix}$            |
| 8.36       | $(E, 0)$                | $\begin{pmatrix} 1'_{a}, 1'_{b} \end{pmatrix}$             |

Table 9. Transformations between type-IV MSG $\mathcal{M}_{\text{std}}$ and conjugated MSGs, where their XSGs are identical to a space group of No. 9 in the ITA standard setting.

| BNS number | Transformation $(P, p)$ | Anti-translations in $(P, p)^{-1}\mathcal{M}_{\text{std}}(P, p)$ |
|------------|------------------------|---------------------------------------------------------------|
| 9.40       | $(E, 0)$                | $\begin{pmatrix} 1'_{c}, 1'_{abc} \end{pmatrix}$            |
|            | $\begin{pmatrix} -1 & 0 & -1 \\ 0 & -1 & 0 \\ 0 & 0 & 1 \end{pmatrix}, \begin{pmatrix} 0 \\ 1/4 \end{pmatrix}$ | $\begin{pmatrix} 1'_{ac}, 1'_{bc} \end{pmatrix}$            |
| 9.41       | $(E, 0)$                | $\begin{pmatrix} 1'_{a}, 1'_{b} \end{pmatrix}$             |
Table 10. Transformations between type-IV MSG $M_{\text{std}}$ and conjugated MSGs, where their XSGs are identical to a space group of No. 10 in the ITA standard setting.

| BNS number | Transformation $(P, p)$ | Anti-translations in $(P, p)^{-1}M_{\text{std}}(P, p)$ |
|------------|-------------------------|------------------------------------------------------|
| 10.47      | $(E, 0)$                | $I'_a$, $I'_c$, $I'_{ac}$                           |
|            | $\begin{pmatrix} -1 & 0 & -1 \\ 0 & -1 & 0 \\ -1 & 0 & 0 \end{pmatrix}$ | $\begin{pmatrix} 0 & -1 & 0 \\ -1 & 0 & 0 \\ 0 & -1 & 0 \end{pmatrix}$ |
| 10.48      | $(E, 0)$                | $I'_b$, $I'_{ab}$                                   |
| 10.49      | $(E, 0)$                | $I'_{ac}$                                           |

Table 11. Transformations between type-IV MSG $M_{\text{std}}$ and conjugated MSGs, where their XSGs are identical to a space group of No. 11 in the ITA standard setting.

| BNS number | Transformation $(P, p)$ | Anti-translations in $(P, p)^{-1}M_{\text{std}}(P, p)$ |
|------------|-------------------------|------------------------------------------------------|
| 11.55      | $(E, 0)$                | $I'_a$, $I'_c$, $I'_{ac}$                           |
|            | $\begin{pmatrix} -1 & 0 & -1 \\ 0 & -1 & 0 \\ -1 & 0 & 0 \end{pmatrix}$ | $\begin{pmatrix} 0 & -1 & 0 \\ -1 & 0 & 0 \\ 0 & -1 & 0 \end{pmatrix}$ |
| 11.56      | $(E, 0)$                | $I'_b$, $I'_{ab}$                                   |
| 11.57      | $(E, 0)$                | $I'_{bc}$                                           |

Table 12. Transformations between type-IV MSG $M_{\text{std}}$ and conjugated MSGs, where their XSGs are identical to a space group of No. 12 in the ITA standard setting.

| BNS number | Transformation $(P, p)$ | Anti-translations in $(P, p)^{-1}M_{\text{std}}(P, p)$ |
|------------|-------------------------|------------------------------------------------------|
| 12.63      | $(E, 0)$                | $I'_{ac}$, $I'_{abc}$                                |
|            | $\begin{pmatrix} -1 & 0 & -1 \\ 0 & -1 & 0 \\ 0 & 0 & 1 \end{pmatrix}$ | $\begin{pmatrix} 0 & -1 & 0 \\ -1 & 0 & 0 \\ 0 & -1 & 0 \end{pmatrix}$ |
| 12.64      | $(E, 0)$                | $I'_{b}$                                            |

In this paper, algorithms for determining magnetic symmetry operations of magnetic crystal structures, identifying magnetic space-group types from a given magnetic space group (MSG), and symmetrizing the magnetic crystal structures on the basis of the determined MSGs are presented.