

Multipole classification in 122 magnetic point groups for unified understanding of multiferroic responses and transport phenomena

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Mutual interplay between the electronic degrees of freedom in solids, such as charge, spin, orbital, sublattice, and bond degrees of freedom, is a source of cross-correlated phenomena with unconventional electronic ordered states. Such degrees of freedom can be described by four types of multipoles (electric, magnetic, magnetic toroidal, and electric toroidal) in a unified way, which enable us to tightly connect the microscopic degrees of freedom with macroscopic physical responses in a transparent manner. We complete a classification of the multipoles in all 122 magnetic point groups based on group theory. The classification is useful to identify potentially active multipoles, not only in ordinary ferromagnetic and antiferromagnetic orderings but also in exotic orderings breaking time-reversal symmetry, e.g., a loop-current state. Moreover, the classification gives an insight into the microscopic origin of the multiferroic responses and quantum transports. By analyzing response functions up to the second order, we summarize the indispensable multipole moments for various responses, such as the linear magnetoelectric, piezoelectric, and elastic responses, and the nonlinear conductivity and Nernst coefficient. Our results highly promote a further discovery of functional multiferroic materials, guided by the bottom-up material design based on the symmetry-adapted multipoles.

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I. INTRODUCTION

Magnetic orderings have long been studied in which various fascinating phenomena emerge such as the anomalous Hall effect [1], multiferroicity like the magnetoelectric effect [2–7], nonreciprocal transports [8], and so on. In ferromagnetic orderings, for example, the uniform magnetization affects the electron kinetics through the Berry-phase-related mechanism, which results in the anomalous Hall effect, Kerr effect, and Nernst effect [1,9,10]. Meanwhile, antiferromagnetic (AFM) orderings can also give rise to the large anomalous Hall effect even with a negligibly small magnetization [11–13], which have been discussed in the noncoplanar AFM ordering [14], the noncollinear AFM ordering in Mn_3Sn [15–17], and the almost collinear-type AFM ordering in RuO_2 [18,19], κ -type organic compounds [20], γ - FeMn [21], and α - Mn [22] and the magneto-optical effect in LaMO_3 ($M = \text{Cr, Mn, and Fe}$) [23]. These studies suggest that the relation between the magnetic orderings and the electromagnetic responses is nontrivial, and there are potential candidates of functional materials that can be utilized for future spintronics devices.

Symmetry is a powerful tool to connect the magnetic orderings and their physical phenomena [24]. In the case of magnetic materials, the physical properties are classified by group theory, such as the magnetic group (Shubnikov group) [24–29] or the magnetic representation theory [30]. It helps us to investigate the macroscopic physical responses, including the unconventional anomalous Hall effect in the AFM

orderings, as mentioned above. However, it is insufficient to understand the microscopic key parameters for the magnetic responses within the symmetry argument.

One of the promising quantities to connect the microscopic electronic degrees of freedom and the macroscopic physical phenomena is the electronic multipoles [31–35], since the multipole degree of freedom constitutes a complete set for an arbitrary Hilbert space with the charge, spin, and orbital degrees of freedom in electrons [36,37]. The multipoles have been mainly used to describe peculiar atomic electronic degrees of freedom in d - or f -electron systems [31,32,35], e.g., the electric quadrupole in CeB_6 [38–44] and magnetic octupole in NpO_2 [45–50]. Meanwhile, the concept of multipole covers not only the atomic electronic degrees of freedom but also ones over multisites and orbitals, such as the hybrid multipole for the interorbital degrees of freedom between different orbitals [36,37,51], the cluster multipole for the on-site degrees of freedom in a cluster [16,52], the bond multipole for the off-site bond degrees of freedom in a cluster [53,54], and the k multipole for the band modulations and spin splittings in the electronic band structures [33,34]. The microscopic description in terms of the electronic multipole degrees of freedom is useful to understand the macroscopic responses in accordance with crystallographic symmetry [33,34,55–60], such as the magnetoelectric effect in magnetic toroidal dipole orderings, e.g., Cr_2O_3 [61], LiCoPO_4 [62,63], and UNi_4B [64,65], and in magnetic quadrupole orderings, e.g., $\text{Co}_4\text{Nb}_2\text{O}_9$ [66–69], the anomalous Hall effect in magnetic octupole orderings, e.g., Mn_3Sn [15,16], the magnetopiezoelec-

tric effect in magnetic quadrupole/hexadecapole orderings, e.g., $\text{Ba}_{1-x}\text{K}_x\text{Mn}_2\text{As}_2$ [70] and EuMn_2Bi_2 [71], and the magnetostriction effect in magnetic octupole orderings [72,73]. Recent studies also clarified that the multipole description gives a systematic microscopic understanding of the band modulation in AFM orderings [54,74–76], e.g., κ -(BEDT-TTF) $_2\text{Cu}[\text{N}(\text{CN})_2]\text{Cl}$ [74,77] and $\text{Ba}_3\text{MnNb}_2\text{O}_9$ [76,78]. Furthermore, the multipole description has been also applied to analyze the nature of the multipole phase transitions based on the Landau free energy expansion [37,79] and the behavior of the effective hyperfine fields for nuclear magnetic or quadrupole resonance (NMR/NQR) spectra [43,47,80,81].

In this way, the multipole description is essential not only to understand the physical phenomena but also to explore further intriguing physics on the basis of microscopic electronic degrees of freedom. As the multipoles are closely related to the spherical harmonics as shown below, they can be systematically classified into the crystal symmetry. Nevertheless, the classification of multipoles has been performed only for the 32 crystallographic point groups [33], and it is still lacking for the 122 magnetic point groups with the antiunitary time-reversal operation. In the present paper, we complete a multipole classification under the 122 magnetic point groups by using four types of multipoles, electric (E), magnetic (M), electric toroidal (ET), and magnetic toroidal (MT) multipoles. The multipole classification enables us to rearrange any AFM orderings or more exotic orderings, such as nematic, excitonic, and loop-current orderings, into the ferroic multipole orderings. The systematic classification by multipoles has an advantage of understanding the nature of potential order parameters and the relevant multiferroic physical phenomena on the basis of microscopic electronic degrees of freedom. We also discuss the relation between the multipoles and the linear/nonlinear response functions based on the Kubo formula beyond the symmetry analysis.

This paper is organized as follows. In Sec. II we review the expressions of the four types of multipoles. In Sec. III the multipole classification in a magnetic point group is presented by exemplifying a cubic system. We show the active E, ET, M, and an MT multipoles in all magnetic point groups in Sec. IV. In Sec. V the relation between the response tensors and the active multipole moments is discussed based on the group theoretical analysis and the Kubo formula. We summarize the present paper in Sec. VI. In Appendix A we give the cubic and tesseral harmonics used for the multipole expressions. Appendix B represents the unitary subgroup for each black-and-white point group. Appendix C gives the classification tables of multipoles, which is not presented in Sec. III. In Appendix D we review the irreducible corepresentation of the magnetic point group. In Appendix E we summarize the relation between the magnetic point groups and (magnetic) Laue groups. The derivation of the multipole expressions of the response tensors in Sec. V is given in Appendix F. In Appendix G the multipole expressions for the response tensors in the hexagonal and trigonal systems are shown.

II. FOUR TYPES OF MULTIPOLES

The multipole moments are introduced by a multipole expansion of the electric scalar potential $\phi(\mathbf{r})$ and magnetic

TABLE I. Four types of multipoles and their spatial-inversion (\mathcal{P}), time-reversal (\mathcal{T}), and \mathcal{PT} parities. The relevant source fields are also presented.

Type	Notation	\mathcal{P}	\mathcal{T}	\mathcal{PT}	Source
E	Q_{lm}	$(-1)^l$	+1	$(-1)^l$	$\rho_e(\mathbf{j}_m)$
M	M_{lm}	$(-1)^{l+1}$	-1	$(-1)^l$	\mathbf{j}_e
MT	T_{lm}	$(-1)^l$	-1	$(-1)^{l+1}$	\mathbf{j}_e
ET	G_{lm}	$(-1)^{l+1}$	+1	$(-1)^{l+1}$	\mathbf{j}_m

vector potential $\mathbf{A}(\mathbf{r})$ representing a spatial distribution of a source electric charge $\rho_e(\mathbf{r})$ and current $\mathbf{j}_e(\mathbf{r})$ in classical electromagnetism [82–87]. The spatial distribution of $\rho_e(\mathbf{r})$ in $\phi(\mathbf{r})$ leads to an E multipole (time-reversal even polar tensor), while that of $\mathbf{j}_e(\mathbf{r})$ in $\mathbf{A}(\mathbf{r})$ leads to an M multipole (time-reversal odd axial tensor) and an MT multipole (time-reversal odd polar tensor). Furthermore, an ET multipole (time-reversal even axial tensor) is introduced by considering the spatial distribution of a magnetic current $\mathbf{j}_m(\mathbf{r})$ [36,88,89]. These four types of multipoles show the different spatial-inversion and time-reversal parities, as summarized in Table I.

In condensed-matter physics, four types of multipoles can describe a spatial distribution of the electronic charge and spin in the atomic orbitals by using their quantum-mechanical operator expressions as [36,37,79]

$$\hat{Q}_{lm} = -e \sum_j O_{lm}(\mathbf{r}_j), \quad (1)$$

$$\hat{M}_{lm} = -\mu_B \sum_j \mathbf{m}_l(\mathbf{r}_j) \cdot \nabla O_{lm}(\mathbf{r}_j), \quad (2)$$

$$\hat{T}_{lm} = -\mu_B \sum_j \mathbf{t}_l(\mathbf{r}_j) \cdot \nabla O_{lm}(\mathbf{r}_j), \quad (3)$$

$$\hat{G}_{lm} = -e \sum_j \sum_{\alpha\beta} g_l^{\alpha\beta}(\mathbf{r}_j) \nabla_\alpha \nabla_\beta O_{lm}(\mathbf{r}_j), \quad (4)$$

where \hat{Q}_{lm} , \hat{M}_{lm} , \hat{T}_{lm} , and \hat{G}_{lm} denote the E, M, MT, and ET multipoles with the azimuthal quantum number l (rank of multipoles) and magnetic quantum number m , respectively. In Eqs. (1)–(4), $-e$ and $-\mu_B$ are the electron charge and Bohr magneton, respectively, which are taken to be unity hereafter, i.e., $-e, -\mu_B \rightarrow 1$. $O_{lm}(\mathbf{r})$ is related with the spherical harmonics as a function of angle $\hat{\mathbf{r}} = \mathbf{r}/|\mathbf{r}|$, $Y_{lm}(\hat{\mathbf{r}})$, which is given by

$$O_{lm}(\mathbf{r}) = \sqrt{\frac{4\pi}{2l+1}} r^l Y_{lm}^*(\hat{\mathbf{r}}). \quad (5)$$

In the following discussion for the crystallographic system, we adopt the real expressions of O_{lm} following Refs. [79,90] and use the multipole notation as X_0 for monopole ($l=0$), (X_x, X_y, X_z) for dipole ($l=1$), $(X_u, X_v, X_{yz}, X_{zx}, X_{xy})$ for quadrupole ($l=2$), $(X_{xyz}, X_x^\alpha, X_y^\alpha, X_z^\alpha, X_x^\beta, X_y^\beta, X_z^\beta)$ for octupole ($l=3$), and $(X_4, X_{4u}, X_{4v}, X_{4x}^\alpha, X_{4y}^\alpha, X_{4z}^\alpha, X_{4x}^\beta, X_{4y}^\beta, X_{4z}^\beta)$ for hexadecapole ($l=4$) following Ref. [33] (see also Appendix A for their expressions). $\mathbf{m}_l(\mathbf{r}_j)$, $\mathbf{t}_l(\mathbf{r}_j)$, and $g_l^{\alpha\beta}(\mathbf{r}_j)$ represent the magnetic moment, magnetic toroidal moment,

and electric toroidal tensor, respectively, which are expressed as

$$\mathbf{m}_l(\mathbf{r}_j) = \frac{2\mathbf{l}_j}{l+1} + \boldsymbol{\sigma}_j, \quad (6)$$

$$\mathbf{t}_l(\mathbf{r}_j) = \frac{\mathbf{r}_j}{l+1} \times \left(\frac{2\mathbf{l}_j}{l+2} + \boldsymbol{\sigma}_j \right), \quad (7)$$

$$g_l^{\alpha\beta}(\mathbf{r}_j) = m_l^\alpha(\mathbf{r}_j)t_l^\beta(\mathbf{r}_j), \quad (8)$$

where \mathbf{l}_j and $\boldsymbol{\sigma}_j/2$ are the dimensionless orbital and spin angular momentum operators of an electron at \mathbf{r}_j , respectively. The parities with respect to the spatial-inversion and time-reversal operations, \mathcal{P} and \mathcal{T} , for each multipole are given as follows: (\mathcal{P} , \mathcal{T}) = $[(-1)^l, +1]$ for Q_{lm} , $[(-1)^{l+1}, -1]$ for M_{lm} , $[(-1)^l, -1]$ for T_{lm} , and $[(-1)^{l+1}, +1]$ for G_{lm} , which are summarized in Table I. The four types of multipoles constitute a complete set for an arbitrary electronic degree of freedom in the atomic orbitals [36,37,79].

The atomic-scale multipole operators in Eqs. (1)–(4) can also be applied to describe anisotropic distributions in a cluster system with the sublattice degree of freedom, which is termed as a cluster multipole [16,35,52,56,91]. For example, the expressions of M and MT multipoles are obtained by reading \mathbf{r}_j in Eqs. (2) and (3) with the position of the j th atom \mathbf{R}_j in a magnetic unit cell. By adopting the virtual atomic cluster method in Ref. [52], one can systematically describe any N -site magnetic structures in terms of cluster M and MT multipoles as follows:

$$\hat{M}_{lm}^{(c)} = \sum_{j=1}^N \boldsymbol{\sigma}_j \cdot \nabla_j O_{lm}(\mathbf{R}_j), \quad (9)$$

$$\hat{T}_{lm}^{(c)} = \frac{1}{l+1} \sum_{j=1}^N (\hat{\mathbf{R}}_j \times \boldsymbol{\sigma}_j) \cdot \nabla_j O_{lm}(\mathbf{R}_j), \quad (10)$$

where the superscript (c) is introduced to represent cluster multipoles for clarity and $\hat{\mathbf{R}}_j = \mathbf{R}_j/|\mathbf{R}_j|$. Equations (9) and (10) give the multipole order parameters under the AFM orderings, which provide an understanding of physical phenomena. For example, the magnetostriction effect under the all-in-all-out magnetic ordering in the pyrochlore structure is understood by the emergence of the cluster M octupole [72] and the linear magnetoelectric effect in the zigzag chain is owing to the active cluster MT dipole [92–94].

III. IRREDUCIBLE REPRESENTATIONS OF MULTIPOLES UNDER MAGNETIC POINT GROUPS

The four types of multipoles in Eqs. (1)–(4) express arbitrary electronic degrees of freedom in the Hilbert space spanned by the electron wave functions in the 32 point-group irreducible representations [33]. In this section we generalize the multipole classification from the 32 crystallographic point groups to the 122 magnetic point groups by taking into account the antiunitary time-reversal operation θ .

The 122 magnetic point groups are categorized into three groups [95]:

- (I) ordinary crystallographic point groups without θ (32),
- (II) gray point groups (32),
- (III) black-and-white point groups (58),

TABLE II. Irreducible corepresentations (IRREP) of magnetic (M) and magnetic toroidal (MT) multipoles ($l \leq 4$) in the cubic gray point group $m\bar{3}m1'$. The superscript “–” of the IRREP means the odd parity with respect to the time-reversal operation. The corresponding magnetic point group (MPG) with its primary axis (P. axis) is also shown.

IRREP	MT	M	MPG	P. axis
A_{1g}^-	T_0, T_4		$m\bar{3}m$	(100)
A_{2g}^-		M_{xyz}	$m\bar{3}m'$	(100)
E_g^-	T_u, T_{4u}		$4/mmm$	[001]
	T_v, T_{4v}		$4'/mmm'$	[001]
T_{1g}^-	T_{4x}^α	M_x, M_x^α	$4/m'm'm'$	[100]
	T_{4y}^α	M_y, M_y^α	$4/m'm'm'$	[010]
	T_{4z}^α	M_z, M_z^α	$4/m'm'm'$	[001]
T_{2g}^-	T_{yz}, T_{4x}^β	M_x^β	$4'/m'm'm$	[100]
	T_{zx}, T_{4y}^β	M_y^β	$4'/m'm'm$	[010]
	T_{xy}, T_{4z}^β	M_z^β	$4'/m'm'm$	[001]
A_{1u}^-		M_0, M_4	$m'\bar{3}'m'$	(100)
A_{2u}^-	T_{xyz}		$m'\bar{3}'m'$	(100)
E_u^-		M_u, M_{4u}	$4'/m'm'm'$	[001]
		M_v, M_{4v}	$4'/m'm'm$	[001]
T_{1u}^-	T_x, T_x^α	M_{4x}^α	$4'/m'm'm$	[100]
	T_y, T_y^α	M_{4y}^α	$4'/m'm'm$	[010]
	T_z, T_z^α	M_{4z}^α	$4'/m'm'm$	[001]
T_{2u}^-	T_x^β	M_{yz}, M_{4x}^β	$4'/m'm'm'$	[100]
	T_y^β	M_{zx}, M_{4y}^β	$4'/m'm'm'$	[010]
	T_z^β	M_{xy}, M_{4z}^β	$4'/m'm'm'$	[001]

where the numbers in parentheses represent the number of magnetic point groups. Supposing \mathbf{G} represents any point group belonging to the type-(I) crystallographic point groups, the type-(II) gray point group, $\mathbf{M}^{(II)}$, is defined so as to contain the double elements of \mathbf{G} , which is represented by

$$\mathbf{M}^{(II)} = \mathbf{G} + \theta\mathbf{G}. \quad (11)$$

Meanwhile, the type-(III) black-and-white point group, $\mathbf{M}^{(III)}$, consists of half of the elements of $\mathbf{M}^{(II)}$, which is represented as

$$\mathbf{M}^{(III)} = \mathbf{H} + \theta(\mathbf{G} - \mathbf{H}), \quad (12)$$

where \mathbf{H} is a halving unitary subgroup of \mathbf{G} . The correspondence between $\mathbf{M}^{(III)}$ and \mathbf{H} in each black-and-white point group is shown in Table XV in Appendix B.

On the basis of the group theory, we classify four types of multipoles under 122 magnetic point groups. We focus on the multipole classification under the magnetic point groups with time-reversal operations, i.e., type-(II) and type-(III) groups. First, let us classify the multipoles under the 32 type-(II) gray point groups, which is summarized in Table II in this section and Tables XVII–XXVI in Appendix C 1. In the following we show the example by taking the cubic gray point group $m\bar{3}m1'$ in Table II.

Table II presents the M and MT multipoles up to rank 4, classified into the irreducible corepresentation under the cubic gray point group $m\bar{3}m1'$. In the table, the superscript “–”

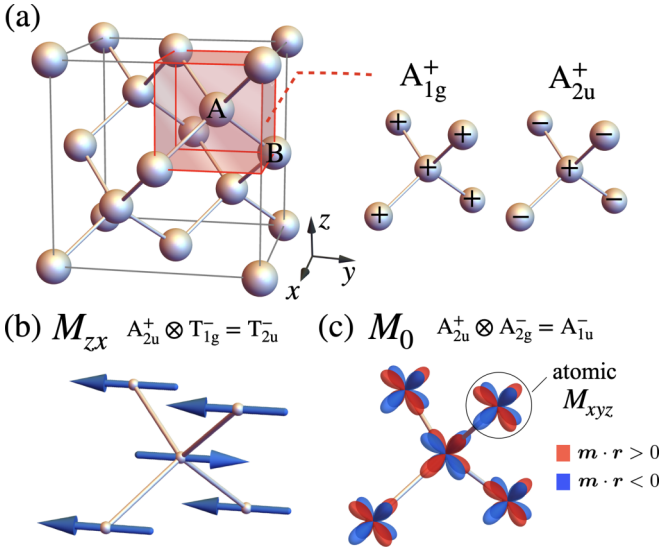


FIG. 1. (a) Diamond structure with two sublattices A and B (left panel). The IRREPs and the corresponding potential distributions in the two sublattices are shown in the right panel. (b) The staggered magnetic dipole along y axis and (c) the staggered xyz -type magnetic octupole, which are regarded as the cluster M quadrupole M_{zx} and the M monopole M_0 , respectively. The arrows in (b) represent the spin direction, and the color in (c) represents the distribution of the magnetic monopole charge defined by $m \cdot r$.

in the IRREP stands for the odd time-inversion property, as discussed in detail in Appendix D. The IRREPs of the E and ET multipoles are obtained by replacing $(T, M) \rightarrow (Q, G)$ and $\Gamma^- \rightarrow \Gamma^+$, where $\Gamma = A_{1g/u}, A_{2g/u}, E_{g/u}, T_{1g/u}, T_{2g/u}$. Table II also shows the reduction to the subgroups in each IRREP. In the table, ‘‘P. axis’’ stands for the primary axis of the point-group operations. For example, the symmetry operations of $4/m\bar{m}m'$ with the P. axis [001] are

$$E, C_{4z}, C_{4z}^3, C_{4z}^2, \theta C'_{2y}, \theta C'_{2y}, \theta C''_{2[110]}, \theta C''_{2[\bar{1}10]}, \quad (13)$$

$$I, IC_{4z}, IC_{4z}^3, \sigma_{\perp z}, \theta \sigma_{\perp x}, \theta \sigma_{\perp y}, \theta \sigma_{\perp[110]}, \theta \sigma_{\perp[\bar{1}10]},$$

where we specify the operation axis or plane in the subscript. On the other hand, for $4/m\bar{m}m'$ with P. axis [100], the operation axes and planes are transformed in cyclic accordance with the change of the P. axis, which is represented as

$$E, C_{4x}, C_{4x}^3, C_{4x}^2, \theta C'_{2y}, \theta C'_{2z}, \theta C''_{2[011]}, \theta C''_{2[0\bar{1}1]}, \quad (14)$$

$$I, IC_{4x}, IC_{4x}^3, \sigma_{\perp x}, \theta \sigma_{\perp y}, \theta \sigma_{\perp z}, \theta \sigma_{\perp[011]}, \theta \sigma_{\perp[0\bar{1}1]}.$$

The classification in Table II provides the identification of hidden/unknown multipole order parameters in a systematic way. Let us take an example of the diamond structure in Fig. 1(a) with the two sublattices A and B under the space group $Fd\bar{3}m$ and the magnetic point group $m\bar{3}m1'$ [96]. Supposing the two-sublattice ordering, the IRREPs for the sublattice degree of freedom, Γ_{sub} , are given by

$$\Gamma_{\text{sub}} = A_{1g}^+ \oplus A_{2u}^+, \quad (15)$$

where A_{1g}^+ corresponds to the uniform potential distribution and A_{2u}^+ corresponds to the staggered one, as shown in the right panel of Fig. 1(a).

When the two-sublattice magnetic order occurs, one can obtain the IRREPs with a total of six components by taking the product of Γ_{sub} and the IRREPs for the M dipole (M_x, M_y, M_z) , $\Gamma_{M1} = T_{1g}^-$, which are represented by [97]

$$\Gamma_{\text{sub}} \otimes \Gamma_{M1} = T_{1g}^- \oplus T_{2u}^-. \quad (16)$$

The IRREP T_{1g}^- in the right-hand side represents the uniform alignment of the M dipole, i.e., the ferromagnetic order. On the other hand, the IRREP T_{2u}^- , which corresponds to the staggered magnetic structure shown in Fig. 1(b), is regarded as the M quadrupole ordering from Table II [98]. Thus it is easy to predict the emergent physical phenomena related with the M quadrupole, such as the transverse magnetoelectric effect, once the staggered magnetic ordering occurs in the diamond structure [99] (see also Sec. V).

Similarly, the classification in Table II is used not only for the AFM ordering but also for the unconventional electronic orderings, such as the spin nematics [100–103], excitonic states [104–109], staggered flux states [110–113], loop-current states [53,54,114–117], and other higher-rank multipole orderings [31,32,52]. For instance, when considering the orderings of the atomic M octupoles $(M_{xyz}, M_x^\alpha, M_y^\alpha, M_z^\alpha, M_x^\beta, M_y^\beta, M_z^\beta)$ with the IRREPs $\Gamma_{M3} = A_{2g}^- \oplus T_{1g}^- \oplus T_{2g}^-$, the possible IRREPs within the two sublattices are given by

$$\Gamma_{\text{sub}} \otimes \Gamma_{M3} = (A_{2g}^- \oplus T_{1g}^- \oplus T_{2g}^-) \oplus (A_{1u}^- \oplus T_{1u}^- \oplus T_{2u}^-). \quad (17)$$

The former (latter) parenthesis represents the uniform (staggered) alignment of M octupoles. From Table II one can find the multipole order parameters, e.g., the staggered M_{xyz} ordering with A_{1u}^- , is regarded as the M monopole M_0 , as schematically shown in Fig. 1(c). Then the staggered M_{xyz} ordering is expected to exhibit physical phenomena in the presence of M_0 , such as the longitudinal magnetoelectric effect.

Next we classify four types of multipoles under the type-(III) black-and-white point groups. The results are summarized in Table III in this section and Tables XXXVII–XXXIV in Appendix C 2. We here show the multipole classification under the maximum subgroups of $m\bar{3}m1'$, among which do not have the time-reversal symmetry, in Table III. The IRREPs in Table III present the transformation property with respect to their unitary subgroup, and the \pm symbol stands for the parity with respect to the antiunitary operation, except for the $B_{2g/u}$ representation of $4'/mmm'$ (see also the discussion in Appendix D).

Table III provides a complete correspondence of the IRREPs for the group-subgroup relation. For example, in the staggered M_{xyz} -type octupole ordering as exemplified above in Fig. 1(c), the symmetry reduces as $m\bar{3}m1' \rightarrow m'\bar{3}'m'$. In this case, the IRREPs of the parent point group $m\bar{3}m1'$ are read by those of the subgroup $m'\bar{3}'m'$ as follows: $(A_{1g}^\pm, A_{1u}^\pm) \rightarrow A_1^\pm$, $(A_{2g}^\pm, A_{2u}^\pm) \rightarrow A_2^\pm$, $(E_g^\pm, E_u^\pm) \rightarrow E^\pm$, $(T_{1g}^\pm, T_{1u}^\pm) \rightarrow T_1^\pm$, $(T_{2g}^\pm, T_{2u}^\pm) \rightarrow T_2^\pm$. Since some of the multipoles are turned to belong to the same IRREP by lowering the symmetry, additional cross couplings between multipoles that are not present in the parent point group are expected, e.g., the

TABLE III. IRREPs of the multipoles in the time-reversal breaking maximum subgroups of the gray point group $m\bar{3}m1'$. $\{X_u + iX_v, X_u - iX_v\}$ and $\{X_{4u} + iX_{4v}, X_{4u} - iX_{4v}\}$ ($X = Q$ or G) are the basis of $E_{g/u}^{(1,2)+}$ in $m\bar{3}m'$, while $\{X_u + iX_v, -X_u + iX_v\}$ and $\{X_{4u} + iX_{4v}, -X_{4u} + iX_{4v}\}$ ($X = T$ or M) for $E_{g/u}^{(1,2)-}$. $\{X_x + iX_y, X_x - iX_y\}$, $\{X_{yz} - iX_{zx}, X_{yz} + iX_{zx}\}$, $\{X_x^\alpha + iX_y^\alpha, X_x^\alpha - iX_y^\alpha\}$, $\{X_x^\beta - iX_y^\beta, X_x^\beta + iX_y^\beta\}$, $\{X_{4x}^\alpha + iX_{4y}^\alpha, X_{4x}^\alpha - iX_{4y}^\alpha\}$, and $\{X_{4x}^\beta - iX_{4y}^\beta, X_{4x}^\beta + iX_{4y}^\beta\}$ ($X = Q, G, T, M$) are the basis of $E_{g/u}^{(1,2)\pm}$ in $4/mmm'$. The IRREPs stand for the transformation property in the unitary subgroups shown in the second row. The superscript \pm of the IRREPs represents the parity with respect to the antiunitary operation in the third row, whose operation axis is shown in the fourth row.

Magnetic point group		$m\bar{3}m1'$	$m\bar{3}m$	$m\bar{3}m'$	$m'\bar{3}'m'$	$m'\bar{3}'m$	$4/mmm$	$4'/mmm'$	$4/mm'm'$	$4/m'm'm'$	$4'/m'm'm$	$4/m'mm$
Unitary subgroup		$m\bar{3}m$		$m\bar{3}$	432	$\bar{4}3m$		mmm	$4/m$	422	$\bar{4}2m$	$4mm$
Antiunitary operation		θ		$\theta C_2'$ [110]	θI	θI		$\theta C_2''$ [110]	$\theta C_2'$ [100]	θI	θI	θI
E	ET											
Q_0, Q_4		A_{1g}^+	A_{1g}	A_g^+	A_1^+	A_1^+	A_{1g}	A_g^+	A_g^+	A_1^+	A_1^+	A_1^+
	G_{xyz}	A_{2g}^+	A_{2g}	A_g^-	A_2^+	A_2^+	B_{1g}	A_g^-	B_g^+	B_1^+	B_1^+	B_1^+
Q_u, Q_{4u}		E_g^+	E_g	$E_g^{(1,2)+}$	E^+	E^+	A_{1g}	A_g^+	A_g^+	A_1^+	A_1^+	A_1^+
Q_v, Q_{4v}							B_{1g}	A_g^-	B_g^+	B_1^+	B_1^+	B_1^+
Q_{4x}^α	G_x, G_x^α	T_{1g}^+	T_{1g}	T_g^+	T_1^+	T_1^+	E_g	B_{2g}	$E_g^{(1,2)+}$	E^+	E^+	E^+
Q_{4y}^α	G_y, G_y^α											
Q_{4z}^α	G_z, G_z^α						A_{2g}	B_{1g}^-	A_g^-	A_2^+	A_2^+	A_2^+
Q_{yz}, Q_{4x}^β	G_x^β	T_{2g}^+	T_{2g}	T_g^-	T_2^+	T_2^+	E_g	B_{2g}	$E_g^{(1,2)+}$	E^+	E^+	E^+
Q_{zx}, Q_{4y}^β	G_y^β											
Q_{xy}, Q_{4z}^β	G_z^β						B_{2g}	B_{1g}^+	B_g^-	B_2^+	B_2^+	B_2^+
	G_0, G_4	A_{1u}^+	A_{1u}	A_u^+	A_1^-	A_2^-	A_{1u}	A_u^+	A_u^+	A_1^-	B_1^-	A_2^-
Q_{xyz}		A_{2u}^+	A_{2u}	A_u^-	A_2^-	A_1^-	B_{1u}	A_u^-	B_u^+	B_1^-	A_1^-	B_2^-
	G_u, G_{4u}	E_u^+	E_u	$E_u^{(1,2)+}$	E^-	E^-	A_{1u}	A_u^+	A_u^+	A_1^-	B_1^-	A_2^-
	G_v, G_{4v}						B_{1u}	A_u^-	B_u^+	B_1^-	A_1^-	B_2^-
Q_x, Q_x^α	G_{4x}^α	T_{1u}^+	T_{1u}	T_u^+	T_1^-	T_2^-	E_u	B_{2u}	$E_u^{(1,2)+}$	E^-	E^-	E^-
Q_y, Q_y^α	G_{4y}^α											
Q_z, Q_z^α	G_{4z}^α						A_{2u}	B_{1u}^-	A_u^-	A_2^-	B_2^-	A_1^-
Q_x^β	G_{yz}, G_{4x}^β	T_{2u}^+	T_{2u}	T_u^-	T_2^-	T_1^-	E_u	B_{2u}	$E_u^{(1,2)+}$	E^-	E^-	E^-
Q_y^β	G_{zx}, G_{4y}^β											
Q_z^β	G_{xy}, G_{4z}^β						B_{2u}	B_{1u}^+	B_u^-	B_2^-	A_2^-	B_1^-
MT	M											
T_0, T_4		A_{1g}^-	A_{1g}	A_g^-	A_1^-	A_1^-	A_{1g}	A_g^-	A_g^-	A_1^-	A_1^-	A_1^-
	M_{xyz}	A_{2g}^-	A_{2g}	A_g^+	A_2^-	A_2^-	B_{1g}	A_g^+	B_g^-	B_1^-	B_1^-	B_1^-
T_u, T_{4u}		E_g^-	E_g	$E_g^{(1,2)-}$	E^-	E^-	A_{1g}	A_g^-	A_g^-	A_1^-	A_1^-	A_1^-
T_v, T_{4v}							B_{1g}	A_g^+	B_g^-	B_1^-	B_1^-	B_1^-
T_{4x}^α	M_x, M_x^α	T_{1g}^-	T_{1g}	T_g^-	T_1^-	T_1^-	E_g	B_{2g}	$E_g^{(1,2)-}$	E^-	E^-	E^-
T_{4y}^α	M_y, M_y^α											
T_{4z}^α	M_z, M_z^α						A_{2g}	B_{1g}^+	A_g^+	A_2^-	A_2^-	A_2^-
T_{yz}, T_{4x}^β	M_x^β	T_{2g}^-	T_{2g}	T_g^+	T_2^-	T_2^-	E_g	B_{2g}	$E_g^{(1,2)-}$	E^-	E^-	E^-
T_{zx}, T_{4y}^β	M_y^β											
T_{xy}, T_{4z}^β	M_z^β						B_{2g}	B_{1g}^-	B_g^+	B_2^-	B_2^-	B_2^-
	M_0, M_4	A_{1u}^-	A_{1u}	A_u^-	A_1^+	A_2^+	A_{1u}	A_u^-	A_u^-	A_1^+	B_1^+	A_2^+
T_{xyz}		A_{2u}^-	A_{2u}	A_u^+	A_2^+	A_1^+	B_{1u}	A_u^+	B_u^-	B_1^+	A_1^+	B_2^+
	M_u, M_{4u}	E_u^-	E_u	$E_u^{(1,2)-}$	E^+	E^+	A_{1u}	A_u^-	A_u^-	A_1^+	B_1^+	A_2^+
	M_v, M_{4v}						B_{1u}	A_u^+	B_u^-	B_1^+	A_1^+	B_2^+
T_x, T_x^α	M_{4x}^α	T_{1u}^-	T_{1u}	T_u^-	T_1^+	T_2^+	E_u	B_{2u}	$E_u^{(1,2)-}$	E^+	E^+	E^+
T_y, T_y^α	M_{4y}^α											
T_z, T_z^α	M_{4z}^α						A_{2u}	B_{1u}^+	A_u^+	A_2^+	B_2^+	A_1^+
T_x^β	M_{yz}, M_{4x}^β	T_{2u}^-	T_{2u}	T_u^+	T_2^+	T_1^+	E_u	B_{2u}	$E_u^{(1,2)-}$	E^+	E^+	E^+
T_y^β	M_{zx}, M_{4y}^β											
T_z^β	M_{xy}, M_{4z}^β						B_{2u}	B_{1u}^-	B_u^+	B_2^+	A_2^+	B_1^+

TABLE IV. Active multipoles in the crystallographic point group (CPG), gray point group (GPG), and black-and-white point group (BWPG) according to \mathcal{P} , \mathcal{T} , and \mathcal{PT} symmetries. “Even/Odd-parity” represents the spatial-inversion parity of multipoles.

Type	Magnetic point group	\mathcal{P}	\mathcal{T}	\mathcal{PT}	Even-parity	Odd-parity	Even-parity	Odd-parity
					E, ET	E, ET	MT, M	MT, M
(I) CPG	$m\bar{3}m, m\bar{3}, 4/mmm, 4/m, mmm, 2/m, \bar{1},$ $6/mmm, 6/m, \bar{3}m, \bar{3}$	○	×	×	✓		✓	
	432, $\bar{4}3m, 23, 422, \bar{4}2m, 4mm, 4, \bar{4}, 222, mm2, 2, m, 1,$ $622, \bar{6}m2, 6mm, 6, \bar{6}, 32, 3m, 3$	×	×	×	✓	✓	✓	✓
(II) GPG	$m\bar{3}m1', m\bar{3}1', 4/mmm1', 4/m1', mmm1', 2/m1', \bar{1}1',$ $6/mmm1', 6/m1', \bar{3}m1', \bar{3}1'$	○	○	○	✓			
	4321', $\bar{4}3m1', 231', 4221', \bar{4}2m1', 4mm1', 41', \bar{4}1',$ $2221', mm21', 21', m1', 11',$ $6221', \bar{6}m21', 6mm1', 61', \bar{6}1', 321', 3m1', 31'$	×	○	×	✓	✓		
	$m\bar{3}m', 4/mm'm', 4'/mm'm, 4'/m, m'm'm, 2'/m',$ $6'/mm'm', 6'/m'mm', 6'/m', \bar{3}m'$	○	×	×	✓		✓	
(III) BWPG	$m'\bar{3}m', m'\bar{3}'m, m'\bar{3}', 4/m'm'm', 4'/m'm'm, 4'/m'mm, 4'/m', 4'/m',$ $m'm'm', m'mm, 2'/m, 2'/m', \bar{1}',$ $6'/m'm'm', 6'/mmm', 6'/m'mm, 6'/m, 6'/m', \bar{3}'m', \bar{3}'m, \bar{3}'$	×	×	○	✓			✓
	4'32', $\bar{4}'3m', 42'2', 4'22', \bar{4}'2m', \bar{4}'2m', \bar{4}'2'm, 4m'm', 4'm'm, 4', \bar{4}',$ $2'2'2, m'm'2, m'm2', 2', m',$ $62'2', 6'22', \bar{6}'m'2', \bar{6}'m2', \bar{6}'m2', 6m'm', 6', \bar{6}', 32', 3m'$	×	×	×	✓	✓	✓	✓

coupling between the MT dipole (T_x, T_y, T_z) and the ET dipole (G_x, G_y, G_z) appears because of the same IRREP T_1^+ .

IV. ACTIVE MULTIPOLES UNDER MAGNETIC POINT GROUPS

In this section we focus on the active multipoles, which belong to the totally symmetric IRREP in each magnetic point group. The active multipoles are roughly classified according to the spatial and time inversion properties in each magnetic point group, as shown in Table IV. The E and ET multipoles can be active for all the magnetic point groups, while the M and MT multipoles can become active only for the type-(I) crystallographic point groups and type-(III) black-and-white point groups without the pure time-reversal symmetry.

Let us start by discussing the active multipoles under type-(I) crystallographic point groups, where not only E and ET multipoles but also M and MT multipoles become active because of the time-reversal symmetry breaking. The type of active multipoles depends on the spatial parity, as shown in Table IV. In the 11 crystallographic point groups with the spatial-inversion symmetry $m\bar{3}m, m\bar{3}, 4/mmm, 4/m, mmm, 2/m, \bar{1}, 6/mmm, 6/m, \bar{3}m,$ and $\bar{3}$, even-parity E, ET, M, and MT multipoles are active. The active multipoles in each crystallographic point group are shown in Table V. On the other hand, in the 21 noncentrosymmetric crystallographic point groups 432, $\bar{4}3m, 23, 422, \bar{4}2m, 4mm, 4, \bar{4}, 222, mm2, 2, m, 1, 622, \bar{6}m2, 6mm, 6, \bar{6}, 32, 3m,$ and 3 , odd-parity E, ET, M, and MT multipoles become active in addition to the even-parity ones, which are shown in Table VI. It is noted that the active E and MT (ET and M) multipoles have the same angle dependence; the same components of Q_{lm} and T_{lm} (G_{lm} and M_{lm}) are activated simultaneously. This is because the type-(I) crystallographic point group has no point-group oper-

ations accompanied by the time-reversal operation. Different from type-(II) and type-(III) magnetic point groups, the MT monopole T_0 is active in the type-(I) crystallographic point group.

In the case of the type-(II) gray point groups, no M and MT multipoles are activated because of the presence of the time-reversal symmetry [33]. The even-parity E and ET multipoles become active in all the type-(II) gray point groups, while the odd-parity E and ET ones become active in the noncentrosymmetric 21 point groups: 4321', $\bar{4}3m1', 231', 4221', \bar{4}2m1', 4mm1', 41', \bar{4}1', 2221', mm21', 21', m1', 11', 6221', \bar{6}m21', 6mm1', 61', \bar{6}1', 321', 3m1',$ and $31'$. The active even-parity E and ET multipoles with rank 0–4 in the centrosymmetric 11 gray point groups are summarized in Table VII. Meanwhile, the E and ET multipoles in the noncentrosymmetric 21 gray point groups are shown in Table VIII.

In the type-(III) black-and-white point groups, four types of multipoles can become active, similar to the type-(I) crystallographic point groups. However, there is a major difference in the symmetry operations; there are proper product operations of the point-group and time-reversal operations in the type-(III) black-and-white point groups, resulting in no relations between the active E and MT (ET and M) multipoles. Thus, the type-(III) black-and-white point groups are classified into three types according to the presence/absence of the \mathcal{P} and \mathcal{PT} symmetries. The first one is the 10 black-and-white point groups with $(\mathcal{P}, \mathcal{PT}) = (\circ, \times), m\bar{3}m', 4/mm'm', 4'/mm'm, 4'/m, m'm'm, 2'/m', 6'/mm'm', 6'/m'mm', 6'/m',$ and $\bar{3}m'$, where the even-parity E, ET, M, and MT multipoles are active, as listed in Table IX. The second one is the 21 black-and-white point groups with $(\mathcal{P}, \mathcal{PT}) = (\times, \circ), m'\bar{3}'m', m'\bar{3}'m, m'\bar{3}', 4/m'm'm', 4'/m'm'm, 4'/m'mm, 4'/m', 4'/m', m'm'm', m'mm, 2'/m, 2'/m', \bar{1}', 6'/m'm'm', 6'/mmm', 6'/m'mm, 6'/m, 6'/m', \bar{3}'m', \bar{3}'m,$ and $\bar{3}'$, where the even-parity

TABLE V. Active even-parity E, ET, MT, and M multipoles in the centrosymmetric crystallographic point groups. The triclinic point group $\bar{1}$ (C_i), in which all the even-parity multipoles are active, is omitted.

	Even-parity					Even-parity				
	E			ET		MT			M	
	$l = 0$	2	4	1	3	0	2	4	1	3
$m\bar{3}m$ (O_h)	Q_0		Q_4			T_0		T_4		
$m\bar{3}$ (T_h)	Q_0		Q_4		G_{xyz}	T_0		T_4		M_{xyz}
$4/mmm$ (D_{4h})	Q_0	Q_u	Q_4, Q_{4u}			T_0	T_u	T_4, T_{4u}		
$4/m$ (C_{4h})	Q_0	Q_u	$Q_4, Q_{4u}, Q_{4z}^\alpha$	G_z	G_z^α	T_0	T_u	$T_4, T_{4u}, T_{4z}^\alpha$	M_z	M_z^α
mmm (D_{2h})	Q_0	Q_u, Q_v	Q_4, Q_{4u}, Q_{4v}		G_{xyz}	T_0	T_u, T_v	T_4, T_{4u}, T_{4v}		M_{xyz}
$2/m$ (C_{2h})	Q_0	Q_u, Q_v, Q_{zx}	$Q_4, Q_{4u}, Q_{4v}, Q_{4y}^\alpha, Q_{4y}^\beta$	G_y	$G_{xyz}, G_y^\alpha, G_y^\beta$	T_0	T_u, T_v, T_{zx}	$T_4, T_{4u}, T_{4v}, T_{4y}^\alpha, T_{4y}^\beta$	M_y	$M_{xyz}, M_y^\alpha, M_y^\beta$
$6/mmm$ (D_{6h})	Q_0	Q_u	Q_{40}			T_0	T_u	T_{40}		
$6/m$ (C_{6h})	Q_0	Q_u	Q_{40}	G_z	G_z^α	T_0	T_u	T_{40}	M_z	M_z^α
$\bar{3}m$ (D_{3d})	Q_0	Q_u	Q_{40}, Q_{4b}		G_{3b}	T_0	T_u	T_{40}, T_{4b}		M_{3b}
$\bar{3}$ (C_{3i})	Q_0	Q_u	Q_{40}, Q_{4a}, Q_{4b}	G_z	$G_{3a}, G_{3b}, G_z^\alpha$	T_0	T_u	T_{40}, T_{4a}, T_{4b}	M_z	$M_{3a}, M_{3b}, M_z^\alpha$

E and ET multipoles and the odd-parity M and MT multipoles become active, as shown in Table X. The last one is the 27 black-and-white point groups with $(\mathcal{P}, \mathcal{PT}) = (\times, \times)$, $4'32'$, $4'3m'$, $42'2'$, $4'22'$, $4'2m'$, $4'2m'$, $4m'm'$, $4'm'm'$, $4'$, $4'$, $2'2'2'$, $m'm'2'$, $m'm'2'$, $2'$, m' , $62'2'$, $6'22'$, $6m'2'$, $6'm'2'$, $6'm'2'$, $6m'm'$, $6'mm'$, $6'$, $6'$, $32'$, and $3m'$, where all types of the multipoles become active irrespective of the spatial-inversion and time-reversal parities, as summarized in Table XI.

Let us remark on the active multipoles from the standpoint of the (magnetic) Laue group, which is often used for the diffraction measurement. The even-parity E and ET multipoles are well classified by 11 Laue groups, $m\bar{3}m$, $m\bar{3}$, $4/mmm$, $4/m$, mmm , $6/mmm$, $6/m$, $\bar{3}m$, $\bar{3}$, $2/m$, and $\bar{1}$, whose correspondence to the magnetic point groups is summarized in Table XXXV in Appendix E. Meanwhile, the even-parity M and MT multipoles are well classified by 32 magnetic Laue groups, $m\bar{3}m1'$, $m\bar{3}1'$, $4/mmm1'$, $4/m1'$, $mmm1'$, $6/mmm1'$, $6/m1'$, $\bar{3}m1'$, $\bar{3}1'$, $2/m1'$, $\bar{1}1'$, $m\bar{3}m$, $m\bar{3}$, $4/mmm$, $4/m$, mmm , $6/mmm$, $6/m$, $\bar{3}m$, $\bar{3}$, $2/m$, $\bar{1}$, $m\bar{3}m'$, $4/mm'm'$, $4'/mm'm'$, $4'/m$, $m'm'm'$, $6'/mm'm'$, $6'/m'mm'$, $6'/m'$, $\bar{3}m'$, and $2'/m'$. The correspondence between the magnetic Laue groups and magnetic point groups is shown in Tables XXXVI and XXXVII in Appendix E.

Tables V–XI are useful to identify what type of ferroic states [118] is realized in a magnetic material, e.g., ferroelectric, ferromagnetic [119–121], ferrotoroidal [122], and ferroelectric toroidal (ferroaxial) states [123], since active E dipole Q_i ($i = x, y, z$), M dipole M_i , MT dipole T_i , and ET dipole G_i correspond to the ferroelectric, ferromagnetic, ferrotoroidal, and ferroaxial order parameters, respectively [124]. One can find all the candidate magnetic point groups with these active dipole moments from Tables V–XI as follows:

(i) E dipole:

$4mm1'$, $41'$, $mm21'$, $6mm1'$, $61'$, $3m1'$, $31'$, $21'$, $m1'$, $11'$, $4mm$, 4 , $mm2$, $6mm$, 6 , $3m$, 3 , 2 , m , 1 , $4m'm'$, $4'm'm'$, $4'$, $m'm'2'$, $m'm'2'$, $6m'm'$, $6'mm'$, $6'$, $3m'$, $2'$, m' ,

(ii) M dipole:

$4/m$, 4 , 4 , $6/m$, $\bar{6}$, 6 , $\bar{3}$, 3 , $\bar{1}$, 1 , $2/m$, 2 , m , $4/mm'm'$, $42'2'$, $4m'm'$, $4'2m'$, $m'm'm'$, $2'2'2'$, $m'm'2'$, $m'm'2'$, $6'/mm'm'$, $62'2'$, $6m'm'$, $6'm'2'$, $\bar{3}m'$, $3m'$, $32'$, $2'/m'$, $2'$, m' ,

(iii) MT dipole:

$4mm$, 4 , $mm2$, $6mm$, 6 , $3m$, 3 , 2 , m , 1 , $4/m'mm$, $4/m'$, mmm' , $6/m'mm$, $6/m'$, $\bar{3}'m$, $\bar{3}'$, $2'/m$, $2/m'$, $\bar{1}'$, $42'2'$, $4'2'm$, $4'$, $2'2'2'$, $m'm'2'$, $62'2'$, $6'm'2'$, $6'$, $32'$, m' , $2'$,

(iv) ET dipole:

$4/m1'$, $41'$, $4'1'$, $6/m1'$, $61'$, $6'1'$, $\bar{3}1'$, $31'$, $2/m1'$, $21'$, $m1'$, $\bar{1}1'$, $11'$, $4/m$, 4 , $\bar{4}$, $6/m$, 6 , $\bar{6}$, $\bar{3}$, 3 , $2/m$, 2 , m , $\bar{1}$, 1 , $4'/m'$, $4/m'$, $4'/m$, $4'$, $\bar{4}'$, $6'/m'$, $6/m'$, $6'/m$, $6'$, $\bar{6}'$, $\bar{3}'$, $2'/m'$, $2/m'$, $2'/m$, $2'$, m' , $\bar{1}'$.

Thus our results contain the previous classification for the ferroelectric, ferromagnetic, ferrotoroidal, and ferroaxial states based on the symmetry analyses [122,125–128]. Furthermore, Tables V–XI provide unconventional order parameters more than the dipole moments, e.g., E/M/MT/ET quadrupole and octupole moments. This classification gives a complete guide to identify the electronic order parameters in a systematic way.

Tables V–XI also enable us to understand the multiferroic phenomena through the couplings between the different multipoles. Let us take an example of the cubic crystal with $m\bar{3}m1'$ symmetry, where the E monopole Q_0 and E hexadecapole Q_4 are active up to rank 4, as shown in Table VII. Once the spontaneous symmetry breaking to $m'\bar{3}'m'$ occurs, magnetic monopole M_0 and magnetic hexadecapole M_4 are additionally activated as shown in Table X.

The identification of active multipoles under the target magnetic point groups enables us to construct the free energy and the Hamiltonian in terms of the multipole degrees of freedom. For example, the Landau free energy expansion can be performed in terms of multipole degrees of freedom for any type of order parameters, which is useful to analyze mutual coupling between them [37,79]. For the above example of the symmetry lowering from $m\bar{3}m1'$ to $m'\bar{3}'m'$, it is easy to notice the additional multipole couplings between (Q_0, Q_4) and (M_0, M_4) , which contribute to the free energy, from the IRREP.

Moreover, one can find the additional active multipoles induced by external fields, such as electric and magnetic fields. For example, when the symmetry is lowered from $m'\bar{3}'m'$ to $4m'm'$ under the magnetic field along the z

TABLE VI. Active E, ET, MT, and M multipoles in the noncentrosymmetric crystallographic point groups. The triclinic point group 1 (C_1), in which all the multipoles are active, is omitted.

	Even-parity						Odd-parity						Even-parity						Odd-parity					
	E			ET			E			ET			MT			M			MT			M		
	$l = 0$	2	4	1	3	1	3	0	2	4	0	2	4	1	3	1	3	1	3	0	2	4		
432 (O)	Q_0		Q_4					G_0		G_4			T_0		T_4							M_0		M_4
$\bar{4}3m$ (T_d)	Q_0		Q_4				Q_{xyz}						T_0		T_4				T_{xyz}					
23 (T)	Q_0		Q_4		G_{xyz}		Q_{xyz}		G_0		G_4		T_0		T_4			M_{xyz}		T_{xyz}		M_0		M_4
422 (D_4)	Q_0	Q_u	Q_4					G_0	G_u	G_4			T_0	T_u	T_4						M_0	M_u	M_4	
			Q_{4u}							G_{4u}					T_{4u}								M_{4u}	
$\bar{4}2m$ (D_{2d})	Q_0	Q_u	Q_4				Q_{xyz}		G_v	G_{4v}			T_0	T_u	T_4					T_{xyz}		M_v	M_{4v}	
			Q_{4u}							G_{4u}					T_{4u}								M_{4u}	
4mm (C_{4v})	Q_0	Q_u	Q_4			Q_z	Q_z^α			G_{4z}^α			T_0	T_u	T_4				T_z	T_z^α			M_{4z}^α	
			Q_{4u}							G_{4u}					T_{4u}								M_{4u}	
4 (C_4)	Q_0	Q_u	Q_4	G_z	G_z^α	Q_z	Q_z^α	G_0	G_u	G_4			T_0	T_u	T_4	M_z	M_z^α	T_z	T_z^α	M_0	M_u	M_4		
			Q_{4u}							G_{4u}					T_{4u}								M_{4u}	
			Q_{4z}^α							G_{4z}^α					T_{4z}^α								M_{4z}^α	
$\bar{4}$ (S_4)	Q_0	Q_u	Q_4	G_z	G_z^α		Q_{xyz}		G_v	G_{4v}			T_0	T_u	T_4	M_z	M_z^α		T_{xyz}		M_v	M_{4v}		
			Q_{4u}				Q_z^β		G_{xy}	G_{4z}^β					T_{4u}				T_z^β		M_{xy}	M_{4z}^β		
			Q_{4z}^α							G_{4z}^α					T_{4z}^α								M_{4z}^α	
222 (D_2)	Q_0	Q_u	Q_4		G_{xyz}		Q_{xyz}	G_0	G_u	G_4			T_0	T_u	T_4			M_{xyz}		T_{xyz}	M_0	M_u	M_4	
		Q_v	Q_{4u}						G_v	G_{4u}				T_v	T_{4u}							M_v	M_{4u}	
			Q_{4v}							G_{4v}					T_{4v}								M_{4v}	
mm2 (C_{2v})	Q_0	Q_u	Q_4		G_{xyz}	Q_z	Q_z^α		G_{xy}	G_{4z}^α			T_0	T_u	T_4			M_{xyz}	T_z	T_z^α		M_{xy}	M_{4z}^α	
		Q_v	Q_{4u}				Q_z^β			G_{4z}^β				T_v	T_{4u}					T_z^β			M_{4z}^β	
			Q_{4v}							G_{4v}					T_{4v}								M_{4v}	
2 (C_2)	Q_0	Q_u	Q_4	G_y	G_{xyz}	Q_y	Q_{xyz}	G_0	G_u	G_4			T_0	T_u	T_4	M_y	M_{xyz}	T_y	T_{xyz}	M_0	M_u	M_4		
		Q_v	Q_{4u}		G_y^α		Q_y^α		G_v	G_{4u}				T_v	T_{4u}			M_y^α	T_y^α		M_v	M_{4u}		
		Q_{zx}	Q_{4v}		G_y^β		Q_y^β		G_{zx}	G_{4v}			T_{zx}	T_{4v}				M_y^β	T_y^β		M_{zx}	M_{4v}		
			Q_{4y}^α							G_{4y}^α					T_{4y}^α								M_{4y}^α	
			Q_{4y}^β							G_{4y}^β					T_{4y}^β								M_{4y}^β	
m (C_s)	Q_0	Q_u	Q_4	G_y	G_{xyz}	Q_z	Q_z^α		G_{xy}	G_{4z}^α			T_0	T_u	T_4	M_y	M_{xyz}	T_z	T_z^α		M_{xy}	M_{4z}^α		
		Q_v	Q_{4u}		G_y^α	Q_x	Q_x^α		G_{yz}	G_{4x}^α				T_v	T_{4u}			M_y^α	T_x^α		M_{yz}	M_{4x}^α		
		Q_{zx}	Q_{4v}		G_y^β		Q_z^β			G_{4z}^β			T_{zx}	T_{4v}				M_y^β	T_z^β			M_{4z}^β		
			Q_{4y}^α				Q_x^β			G_{4x}^β					T_{4y}^α				T_x^β			M_{4x}^β		
			Q_{4y}^β							G_{4x}^β					T_{4y}^β								M_{4x}^β	
622 (D_6)	Q_0	Q_u	Q_{40}					G_0	G_u	G_{40}			T_0	T_u	T_{40}						M_0	M_u	M_{40}	
$\bar{6}m2$ (D_{3h})	Q_0	Q_u	Q_{40}				Q_{3b}			G_{4b}			T_0	T_u	T_{40}				T_{3b}				M_{4b}	
6mm (C_{6v})	Q_0	Q_u	Q_{40}			Q_z	Q_z^α						T_0	T_u	T_{40}				T_z	T_z^α				
6 (C_6)	Q_0	Q_u	Q_{40}	G_z	G_z^α	Q_z	Q_z^α	G_0	G_u	G_{40}			T_0	T_u	T_{40}	M_z	M_z^α	T_z	T_z^α	M_0	M_u	M_{40}		
$\bar{6}$ (C_{3h})	Q_0	Q_u	Q_{40}	G_z	G_z^α		Q_{3a}			G_{4a}			T_0	T_u	T_{40}	M_z	M_z^α		T_{3a}			M_{4a}		
							Q_{3b}			G_{4b}					T_{40}				T_{3b}			M_{4b}		
32 (D_3)	Q_0	Q_u	Q_{40}		G_{3b}		Q_{3b}	G_0	G_u	G_{40}			T_0	T_u	T_{40}			M_{3b}		T_{3b}	M_0	M_u	M_{40}	
			Q_{4b}							G_{4b}					T_{4b}								M_{4b}	
3m (C_{3v})	Q_0	Q_u	Q_{40}		G_{3b}	Q_z	Q_{3a}			G_{4a}			T_0	T_u	T_{40}			M_{3b}	T_z	T_{3a}			M_{4a}	
			Q_{4b}				Q_z^α			G_{4a}					T_{4b}					T_z^α			M_{4a}	
3 (C_3)	Q_0	Q_u	Q_{40}	G_z	G_{3a}	Q_z	Q_{3a}	G_0	G_u	G_{40}			T_0	T_u	T_{40}	M_z	M_{3a}	T_z	T_{3a}	M_0	M_u	M_{40}		
			Q_{4a}		G_{3b}		Q_{3b}			G_{4a}					T_{4a}			M_{3b}		T_{3b}			M_{4a}	
			Q_{4b}		G_z^α		Q_z^α			G_{4b}					T_{4b}			M_z^α		T_z^α			M_{4b}	

axis, H_z , the additional active multipoles up to rank 4, are Q_z , Q_u , Q_z^α , Q_{4u} , G_{4z}^α , M_z , M_u , M_z^α , M_{4u} , and T_{4z}^α , as shown in Table XI. Then the additional multipole couplings by the magnetic field arise, which become a source of the field-

induced multiferroic phenomena. For example, since Q_z and Q_u correspond to the electric polarization P_z and the $(3z^2 - r^2)$ -type symmetric strain ε_u , respectively, one can expect that the magnetoelectric coupling $H_z P_z$ ($M_z Q_z$) and

TABLE VII. Active even-parity E and ET multipoles in the centrosymmetric gray point groups. The triclinic point group $\bar{1}1'$, in which all the even-parity E and ET multipoles are active, is omitted.

	Even-parity				
	E			ET	
	$l = 0$	2	4	1	3
$m\bar{3}m1'$	Q_0		Q_4		
$m\bar{3}1'$	Q_0		Q_4		G_{xyz}
$4/mmm1'$	Q_0	Q_u	Q_4, Q_{4u}		
$4/m1'$	Q_0	Q_u	$Q_4, Q_{4u}, Q_{4z}^\alpha$	G_z	G_z^α
$mmm1'$	Q_0	Q_u, Q_v	Q_4, Q_{4u}, Q_{4v}		G_{xyz}
$2/m1'$	Q_0	Q_u, Q_v, Q_{zx}	$Q_4, Q_{4u}, Q_{4v}, Q_{4y}^\alpha, Q_{4y}^\beta$	G_y	$G_{xyz}, G_y^\alpha, G_y^\beta$
$6/mmm1'$	Q_0	Q_u	Q_{40}		
$6/m1'$	Q_0	Q_u	Q_{40}	G_z	G_z^α
$\bar{3}m1'$	Q_0	Q_u	Q_{40}, Q_{4b}		G_{3b}
$\bar{3}1'$	Q_0	Q_u	Q_{40}, Q_{4a}, Q_{4b}	G_z	$G_{3a}, G_{3b}, G_z^\alpha$

magnetoelastic coupling $H_z \varepsilon_u (M_z Q_u)$ to appear in the free energy expansion.

In addition, our result can be used when constructing the so-called hyperfine coupling to investigate the field dependence of the NQR/NMR spectra [81]. Besides, such multipole couplings in each magnetic point group are also related with the band deformations [54,75,76,129] and field responses [33,34,130]. The latter are discussed in the next section.

V. LINEAR AND NONLINEAR RESPONSES UNDER ACTIVE MULTIPOLE

According to Neumann's principle, macroscopic physical responses are determined not by the space-group symmetry but by the crystallographic point-group symmetry [131,132]. This can be generalized to magnetic point groups: macroscopic responses in magnets, such as the Hall conductivity, the linear magnetoelectric effect, and nonlin-

TABLE VIII. Active E and ET multipoles in the noncentrosymmetric gray point groups. The triclinic point group $11'$, in which all the E and ET multipoles are active, is omitted.

	Even-parity					Odd-parity				
	E			ET		E		ET		
	$l = 0$	2	4	1	3	1	3	0	2	4
$4321'$	Q_0		Q_4					G_0		G_4
$\bar{4}3m1'$	Q_0		Q_4				Q_{xyz}			
$231'$	Q_0		Q_4		G_{xyz}		Q_{xyz}	G_0		G_4
$4221'$	Q_0	Q_u	Q_4, Q_{4u}					G_0	G_u	G_4, G_{4u}
$\bar{4}2m1'$	Q_0	Q_u	Q_4, Q_{4u}				Q_{xyz}		G_v	G_{4v}
$4mm1'$	Q_0	Q_u	Q_4, Q_{4u}			Q_z	Q_z^α			G_{4z}^α
$41'$	Q_0	Q_u	$Q_4, Q_{4u}, Q_{4z}^\alpha$	G_z	G_z^α	Q_z	Q_z^α	G_0	G_u	$G_4, G_{4u}, G_{4z}^\alpha$
$\bar{4}1'$	Q_0	Q_u	$Q_4, Q_{4u}, Q_{4z}^\alpha$	G_z	G_z^α		Q_{xyz}, Q_z^β		G_v, G_{xy}	G_{4v}, G_{4z}^β
$2221'$	Q_0	Q_u, Q_v	Q_4, Q_{4u}, Q_{4v}		G_{xyz}		Q_{xyz}	G_0	G_u, G_v	G_4, G_{4u}, G_{4v}
$mm21'$	Q_0	Q_u, Q_v	Q_4, Q_{4u}, Q_{4v}		G_{xyz}	Q_z	Q_z^α, Q_z^β		G_{xy}	$G_{4z}^\alpha, G_{4z}^\beta$
$21'$	Q_0	Q_u, Q_v, Q_{zx}	$Q_4, Q_{4u}, Q_{4v}, Q_{4y}^\alpha, Q_{4y}^\beta$	G_y	$G_{xyz}, G_y^\alpha, G_y^\beta$	Q_y	$Q_{xyz}, Q_y^\alpha, Q_y^\beta$	G_0	G_u, G_v, G_{zx}	$G_4, G_{4u}, G_{4v}, G_{4y}^\alpha, G_{4y}^\beta$
$m1'$	Q_0	Q_u, Q_v, Q_{zx}	$Q_4, Q_{4u}, Q_{4v}, Q_{4y}^\alpha, Q_{4y}^\beta$	G_y	$G_{xyz}, G_y^\alpha, G_y^\beta$	Q_z, Q_x	$Q_z^\alpha, Q_x^\alpha, Q_z^\beta, Q_x^\beta$		G_{xy}, G_{yz}	$G_{4z}^\alpha, G_{4x}^\alpha, G_{4z}^\beta, G_{4x}^\beta$
$6221'$	Q_0	Q_u	Q_{40}					G_0	G_u	G_{40}
$\bar{6}m21'$	Q_0	Q_u	Q_{40}				Q_{3b}			G_{4b}
$6mm1'$	Q_0	Q_u	Q_{40}			Q_z	Q_z^α			
$61'$	Q_0	Q_u	Q_{40}	G_z	G_z^α	Q_z	Q_z^α	G_0	G_u	G_{40}
$\bar{6}1'$	Q_0	Q_u	Q_{40}	G_z	G_z^α		Q_{3a}, Q_{3b}			G_{4a}, G_{4b}
$321'$	Q_0	Q_u	Q_{40}, Q_{4b}		G_{3b}		Q_{3b}	G_0	G_u	G_{40}, G_{4b}
$3m1'$	Q_0	Q_u	Q_{40}, Q_{4b}		G_{3b}	Q_z	Q_{3a}, Q_z^α			G_{4a}
$31'$	Q_0	Q_u	Q_{40}, Q_{4a}, Q_{4b}	G_z	$G_{3a}, G_{3b}, G_z^\alpha$	Q_z	$Q_{3a}, Q_{3b}, Q_z^\alpha$	G_0	G_u	G_{40}, G_{4a}, G_{4b}

TABLE IX. Active even-parity E, ET, MT, and M multipoles in the centrosymmetric black-and-white point groups.

	Even-parity					Even-parity				
	E			ET		MT			M	
	$l = 0$	2	4	1	3	0	2	4	1	3
$m\bar{3}m'$	Q_0		Q_4							M_{xyz}
$4/m\bar{m}'m'$	Q_0	Q_u	Q_4, Q_{4u}					T_{4z}	M_z	M_z^α
$4'/m\bar{m}m'$	Q_0	Q_u	Q_4, Q_{4u}			T_v		T_{4v}		M_{xyz}
$4'/m$	Q_0	Q_u	$Q_4, Q_{4u}, Q_{4z}^\alpha$	G_z	G_z^α	T_v, T_{xy}		T_{4v}, T_{4z}^β		M_{xyz}, M_z^β
$m'm'm$	Q_0	Q_u, Q_v	Q_4, Q_{4u}, Q_{4v}		G_{xyz}	T_{xy}		$T_{4z}^\alpha, T_{4z}^\beta$	M_z	M_z^α, M_z^β
$2'/m'$	Q_0	Q_u, Q_v, Q_{zx}	$Q_4, Q_{4u}, Q_{4v}, Q_{4y}^\alpha, Q_{4y}^\beta$	G_y	$G_{xyz}, G_y^\alpha, G_y^\beta$	T_{xy}, T_{yz}		$T_{4z}^\alpha, T_{4x}^\alpha, T_{4z}^\beta, T_{4x}^\beta$	M_z, M_x	$M_z^\alpha, M_x^\alpha, M_z^\beta, M_x^\beta$
$6/m\bar{m}'m'$	Q_0	Q_u	Q_{40}						M_z	M_z^α
$6'/m'mm'$	Q_0	Q_u	Q_{40}					T_{4a}		M_{3a}
$6'/m'$	Q_0	Q_u	Q_{40}	G_z	G_z^α			T_{4a}, T_{4b}		M_{3a}, M_{3b}
$\bar{3}m'$	Q_0	Q_u	Q_{40}, Q_{4b}		G_{3b}			T_{4a}	M_z	M_{3a}, M_z^α

ear conductivity, are determined by the magnetic point-group symmetry [24,125,133–138]. In this section we show physical responses under the active multipole in any magnetic point group. The correspondence between the response tensor components and multipoles will provide useful information to systematically discuss the essential microscopic model parameters for the responses in the magnetic materials [130]. First we discuss the relation between the response tensors and multipoles based on the point-group symmetry in Sec. VA. Then we discuss the role of the antiunitary time-reversal

operation on the response function by using the linear and second-order nonlinear response theory in Secs. VB and VC, respectively.

A. Correspondence between tensor component and multipole

First we discuss the relation between the response tensor components and multipoles on the basis of group theory. The response tensor $\chi^{[n_B \times n_F]}$ is defined as

$$B^{[n_B]} = \chi^{[n_B \times n_F]} F^{[n_F]}, \quad (18)$$

TABLE X. Active even-parity E and ET multipoles and odd-parity MT and M multipoles in the noncentrosymmetric black-and-white point groups with the \mathcal{PT} symmetry. The triclinic point group $\bar{1}'$ is omitted, where all the even-parity E and ET multipoles and odd-parity MT and M multipoles are active.

	Even-parity					Odd-parity				
	E			ET		MT			M	
	$l = 0$	2	4	1	3	1	3	0	2	4
$m'\bar{3}'m'$	Q_0		Q_4					M_0		M_4
$m'\bar{3}'m$	Q_0		Q_4				T_{xyz}			
$m'\bar{3}'$	Q_0		Q_4		G_{zyz}		T_{xyz}	M_0		M_4
$4/m'm'm'$	Q_0	Q_u	Q_4, Q_{4u}					M_0	M_u	M_4, M_{4u}
$4'/m'm'm$	Q_0	Q_u	Q_4, Q_{4u}				T_{xyz}		M_v	M_{4v}
$4'/m'mm$	Q_0	Q_u	Q_4, Q_{4u}			T_z	T_z^α			M_{4z}^α
$4'/m'$	Q_0	Q_u	$Q_4, Q_{4u}, Q_{4z}^\alpha$	G_z	G_z^α		T_{xyz}, T_z^β		M_v, M_{xy}	M_{4v}, M_{4z}^β
$4/m'$	Q_0	Q_u	$Q_4, Q_{4u}, Q_{4z}^\alpha$	G_z	G_z^α	T_z	T_z^α	M_0	M_u	$M_4, M_{4u}, M_{4z}^\alpha$
mmm'	Q_0	Q_u, Q_v	Q_4, Q_{4u}, Q_{4v}		G_{xyz}	T_z	T_z^α, T_z^β		M_{xy}	$M_{4z}^\alpha, M_{4z}^\beta$
$m'm'm'$	Q_0	Q_u, Q_v	Q_4, Q_{4u}, Q_{4v}		G_{xyz}		T_{xyz}	M_0	M_u, M_v	M_4, M_{4u}, M_{4v}
$2'/m$	Q_0	Q_u, Q_v, Q_{zx}	$Q_4, Q_{4u}, Q_{4v}, Q_{4y}^\alpha, Q_{4y}^\beta$	G_y	$G_{xyz}, G_y^\alpha, G_y^\beta$	T_z, T_x	$T_z^\alpha, T_x^\alpha, T_z^\beta, T_x^\beta$		M_{xy}, M_{yz}	$M_{4z}^\alpha, M_{4x}^\alpha, M_{4z}^\beta, M_{4x}^\beta$
$2/m'$	Q_0	Q_u, Q_v, Q_{zx}	$Q_4, Q_{4u}, Q_{4v}, Q_{4y}^\alpha, Q_{4y}^\beta$	G_y	$G_{xyz}, G_y^\alpha, G_y^\beta$	T_y	$T_{xyz}, T_y^\alpha, T_y^\beta$	M_0	M_u, M_v, M_{zx}	$M_4, M_{4u}, M_{4v}, M_{4y}^\alpha, M_{4y}^\beta$
$6/m'm'm'$	Q_0	Q_u	Q_{40}					M_0	M_u	M_{40}
$6'/m\bar{m}m'$	Q_0	Q_u	Q_{40}				T_{3b}			M_{4b}
$6'/m'mm$	Q_0	Q_u	Q_{40}			T_z	T_z^α			
$6'/m$	Q_0	Q_u	Q_{40}	G_z	G_z^α		T_{3a}, T_{3b}			M_{4a}, M_{4b}
$6/m'$	Q_0	Q_u	Q_{40}	G_z	G_z^α	T_z	T_z^α	M_0	M_u	M_{40}
$\bar{3}'m'$	Q_0	Q_u	Q_{40}, Q_{4b}		G_{3b}		T_{3b}	M_0	M_u	M_{40}, M_{4b}
$\bar{3}'m$	Q_0	Q_u	Q_{40}, Q_{4b}		G_{3b}	T_z	T_{3a}, T_z^α			M_{4a}
$\bar{3}'$	Q_0	Q_u	Q_{40}, Q_{4a}, Q_{4b}	G_z	$G_{3a}, G_{3b}, G_z^\alpha$	T_z	$T_{3a}, T_{3b}, T_z^\alpha$	M_0	M_u	M_{40}, M_{4a}, M_{4b}

TABLE XI. Active multipoles in the noncentrosymmetric black-and-white point groups without the \mathcal{PT} symmetry.

	Even-parity						Odd-parity						Even-parity						Odd-parity					
	E			ET			E			ET			MT			M			MT			M		
	$l = 0$	2	4	1	3		1	3	0	2	4	0	2	4	1	3	1	3	0	2	4			
$\bar{4}'3m'$	Q_0		Q_4					Q_{xyz}								M_{xyz}			M_0		M_4			
$4'32'$	Q_0		Q_4						G_0		G_4					M_{xyz}		T_{xyz}						
$42'2'$	Q_0	Q_u	Q_4						G_0	G_u	G_4			T_{4z}^α	M_z	M_z^α	T_z	T_z^α			M_{4z}^α			
			Q_{4u}								G_{4u}													
$4'22'$	Q_0	Q_u	Q_4						G_0	G_u	G_4			T_v	T_{4v}	M_{xyz}		T_{xyz}		M_v	M_{4v}			
			Q_{4u}								G_{4u}													
$\bar{4}2'm'$	Q_0	Q_u	Q_4					Q_{xyz}			G_v	G_{4v}			T_{4z}^α	M_z	M_z^α	T_z^β		M_{xy}	M_{4z}^β			
			Q_{4u}								G_v	G_{4v}			T_v	T_{4v}	M_{xyz}		M_0	M_u	M_4			
$\bar{4}2m'$	Q_0	Q_u	Q_4					Q_{xyz}			G_v	G_{4v}			T_v	T_{4v}	M_{xyz}		M_0	M_u	M_4			
			Q_{4u}								G_v	G_{4v}			T_v	T_{4v}	M_{xyz}				M_{4u}			
$\bar{4}m2'$	Q_0	Q_u	Q_4					Q_z^β			G_{xy}	G_{4z}^β			T_v	T_{4v}	M_{xyz}	T_z	T_z^α		M_{4z}^α			
			Q_{4u}								G_{xy}	G_{4z}^β			T_v	T_{4v}	M_{xyz}				M_{4z}^α			
$4m'm'$	Q_0	Q_u	Q_4				Q_z	Q_z^α				G_{4z}^α			T_{4z}^α	M_z	M_z^α		M_0	M_u	M_4			
			Q_{4u}									G_{4z}^α									M_{4u}			
$4'mm'$	Q_0	Q_u	Q_4				Q_z	Q_z^α				G_{4z}^α			T_v	T_{4v}	M_{xyz}	T_z^β		M_{xy}	M_{4z}^β			
			Q_{4u}									G_{4z}^α									M_{4z}^β			
$4'$	Q_0	Q_u	Q_4	G_z	G_z^α		Q_z	Q_z^α	G_0	G_u	G_4			T_v	T_{4v}	M_{xyz}		T_{xyz}		M_v	M_{4v}			
			Q_{4u}								G_{4u}			T_{xy}	T_{4z}^β	M_z^β		T_z^β		M_{xy}	M_{4z}^β			
			Q_{4z}^α								G_{4z}^α										M_{4z}^β			
$\bar{4}'$	Q_0	Q_u	Q_4	G_z	G_z^α		Q_{xyz}				G_v	G_{4v}			T_v	T_{4v}	M_{xyz}	T_z	T_z^α	M_0	M_u	M_4		
			Q_{4u}				Q_z^β				G_{xy}	G_{4z}^β			T_{xy}	T_{4z}^β	M_z^β				M_{4u}	M_{4z}^α		
			Q_{4z}^α								G_{xy}	G_{4z}^β			T_{xy}	T_{4z}^β	M_z^β				M_{4u}	M_{4z}^α		
$2'2'2$	Q_0	Q_u	Q_4		G_{xyz}		Q_{xyz}		G_0	G_u	G_4			T_{xy}	T_{4z}^α	M_z	M_z^α	T_z	T_z^α		M_{xy}	M_{4z}^α		
		Q_v	Q_{4u}							G_v	G_{4u}				T_{4z}^β	M_z^β		T_z^β			M_{4z}^β			
			Q_{4v}								G_{4v}										M_{4z}^β			
$m'm2'$	Q_0	Q_u	Q_4		G_{xyz}		Q_z	Q_z^α		G_{xy}	G_{4z}^α			T_{zx}	T_{4y}^α	M_y	M_y^α	T_x	T_x^α		M_{yz}	M_{4x}^α		
		Q_v	Q_{4u}				Q_z^β				G_{4z}^α				T_{4y}^β	M_y^β		T_x^β			M_{4x}^β			
			Q_{4v}								G_{4z}^α				T_{4y}^β	M_y^β		T_x^β			M_{4x}^β			
$m'm'2$	Q_0	Q_u	Q_4		G_{xyz}		Q_z	Q_z^α		G_{xy}	G_{4z}^α			T_{xy}	T_{4z}^α	M_z	M_z^α	T_{xyz}	M_0	M_u	M_4			
		Q_v	Q_{4u}				Q_z^β				G_{4z}^α				T_{4z}^β	M_z^β				M_v	M_{4u}			
			Q_{4v}								G_{4z}^α										M_{4v}			
m'	Q_0	Q_u	Q_4	G_y	G_{xyz}		Q_z	Q_z^α		G_{xy}	G_{4z}^α			T_{xy}	T_{4z}^α	M_z	M_z^α	T_y	T_{xyz}	M_0	M_u	M_4		
		Q_v	Q_{4u}		G_y^α		Q_x	Q_x^α		G_{yz}	G_{4x}^α			T_{yz}	T_{4x}^α	M_x	M_x^α	T_y^α		M_v	M_{4u}			
			Q_{4v}		G_y^β		Q_x^β				G_{4x}^α				T_{4x}^β	M_x^β		T_y^β		M_{zx}	M_{4v}			
		$Q_{4y}^\alpha, Q_{4y}^\beta$					Q_x^β				G_{4x}^α				T_{4x}^β	M_x^β					$M_{4y}^\alpha, M_{4y}^\beta$			
$2'$	Q_0	Q_u	Q_4	G_y	G_{xyz}		Q_y	Q_{yz}^α	G_0	G_u	G_4			T_{xy}	T_{4z}^α	M_z	M_z^α	T_z	T_z^α		M_{xy}	M_{4z}^α		
		Q_v	Q_{4u}		G_y^α		Q_y^α			G_v	G_{4u}			T_{yz}	T_{4x}^α	M_x	M_x^α	T_x	T_x^α		M_{yz}	M_{4x}^α		
			Q_{4v}		G_y^β		Q_y^β			G_{zx}	G_{4v}				T_{4x}^β	M_x^β		T_z^β			M_{4z}^β			
		$Q_{4y}^\alpha, Q_{4y}^\beta$									$G_{4y}^\alpha, G_{4y}^\beta$				T_{4x}^β	M_x^β		T_x^β			M_{4x}^β			
$62'2'$	Q_0	Q_u	Q_{40}						G_0	G_u	G_{40}					M_z	M_z^α	T_z	T_z^α					
$6'22'$	Q_0	Q_u	Q_{40}						G_0	G_u	G_{40}			T_{4a}		M_{3a}		T_{3a}			M_{4a}			
$\bar{6}m'2'$	Q_0	Q_u	Q_{40}					Q_{3b}			G_{4b}				M_z	M_z^α		T_{3a}			M_{4a}			
$\bar{6}'m'2$	Q_0	Q_u	Q_{40}					Q_{3b}			G_{4b}			T_{4b}		M_{3b}			M_0	M_u	M_{40}			
$\bar{6}'m2'$	Q_0	Q_u	Q_{40}					Q_{3b}			G_{4b}			T_{4a}		M_{3a}		T_z	T_z^α		M_0	M_u	M_{40}	
$6m'm'$	Q_0	Q_u	Q_{40}				Q_z	Q_z^α							M_z	M_z^α			M_0	M_u	M_{40}			
$6'mm'$	Q_0	Q_u	Q_{40}				Q_z	Q_z^α						T_{4a}		M_{3a}		T_{3b}			M_{4b}			
$6'$	Q_0	Q_u	Q_{40}	G_z	G_z^α		Q_z	Q_z^α	G_0	G_u	G_{40}			T_{4a}		M_{3a}		T_{3a}			M_{4a}			
											G_{40}			T_{4b}		M_{3b}		T_{3b}			M_{4b}			
$\bar{6}'$	Q_0	Q_u	Q_{40}	G_z	G_z^α		Q_{3a}				G_{4a}			T_{4a}		M_{3a}		T_z	T_z^α	M_0	M_u	M_{40}		
							Q_{3b}				G_{4b}			T_{4b}		M_{3b}					M_{40}			
$3m'$	Q_0	Q_u	Q_{40}		G_{3b}		Q_z	Q_{3a}			G_{4a}			T_{4a}	M_z	M_{3a}		T_{3b}	M_0	M_u	M_{40}			
			Q_{4b}				Q_z^α				G_{4a}					M_z^α					M_{4b}			
$32'$	Q_0	Q_u	Q_{40}		G_{3b}		Q_{3b}		G_0	G_u	G_{40}			T_{4a}	M_z	M_{3a}		T_{3a}	T_z	T_{3a}	M_{4a}			
			Q_{4b}								G_{4b}					M_z^α		T_z^α			M_{4a}			

TABLE XII. Correspondence of the external fields and the responses to the multipoles. The spatial-inversion parity of the external field or the response is shown in the column of \mathcal{P} . In the column of multipole, X_{lm} means the rank- l multipole ($X = Q, G, M, T, l = 0, 1, 2$).

n_F	\mathcal{P}	External field	Multipole
1	+	Magnetic field \mathbf{H}	M dipole (M_{1m})
	-	Electric field \mathbf{E}	E dipole (Q_{1m})
2	+	(Symmetric) stress $\boldsymbol{\tau}$	E monopole (Q_0) E quadrupole (Q_{2m})
n_B		Response	
1	+	Magnetization \mathbf{M}	M dipole (M_{1m})
		Rotation $\boldsymbol{\omega}$	ET dipole (G_{1m})
	-	Electric polarization \mathbf{P}	E dipole (Q_{1m})
		Electric (Thermal) current $\mathbf{J}(\mathbf{J}^Q)$	MT dipole (T_{1m})
2	+	Symmetric strain $\boldsymbol{\varepsilon}$	E monopole (Q_0) E quadrupole (Q_{2m})
	-	Spin current \mathbf{J}^S	ET monopole (G_0) E dipole (Q_{1m}) ET quadrupole (G_{2m})

where $B^{[n_B]}$ and $F^{[n_F]}$ are the rank- n_B (output) response and the rank- n_F external (input) field, respectively, which are typically represented by the electric, magnetic, elastic, and their product degrees of freedom. For example, $F^{[n_F]}$ is an electric field \mathbf{E} , a magnetic field \mathbf{H} , a (symmetric) stress $\boldsymbol{\tau}$, and their combination, while $B^{[n_B]}$ is the electric polarization \mathbf{P} , magnetization \mathbf{M} , symmetric strain $\varepsilon_{ij} = (\partial_i u_j + \partial_j u_i)/2$, and rotation $\boldsymbol{\omega} = (\nabla \times \mathbf{u})/2$, where \mathbf{u} is the displacement vector [139]. $B^{[n_B]}$ also represents quantities for the transport phenomena, such as the electric (thermal) current \mathbf{J} (\mathbf{J}^Q) and the spin current $J_{ij}^S = \sigma_i J_j$. Each external field and response have the correspondence to the multipoles, e.g., electric field $\mathbf{E} \leftrightarrow$ E dipole and symmetric strain $\boldsymbol{\varepsilon} \leftrightarrow$ E monopole and E quadrupole. The representative relation is summarized in Table XII, where the correspondence between the external field (response) and multipole is shown in the upper (lower) panel.

According to the spatial parities of $B^{[n_B]}$ and $F^{[n_F]}$, $\chi^{[n_B \times n_F]}$ becomes a polar or axial tensor; $\chi^{[n_B \times n_F]}$ is the polar (axial) tensor for the parity $\mathcal{P} = (-1)^{n_B + n_F}$ [$\mathcal{P} = (-1)^{n_B + n_F + 1}$]. In the following, the correspondence between multipoles and rank-1, -2, -3, and -4 tensors are shown in Secs. VA 1–VA 4, respectively. See also Appendix F for details of the derivation. In the following, we mainly focus on the response tensors in cubic, tetragonal, orthorhombic, monoclinic, and triclinic systems, and show those in hexagonal and trigonal systems in Appendix G.

1. Rank-1 tensor

The rank-1 response tensor $\chi^{[0 \times 1]}$ for the scalar response $B^{[0]} = (B)$ with $n_B = 0$ and vector field $F^{[1]} = (F_x, F_y, F_z)$ with $n_F = 1$ is related with the dipole (X_x, X_y, X_z) as

$$\chi^{[0 \times 1]} = (X_x \quad X_y \quad X_z), \quad (19)$$

where X stands for the polar multipoles (Q or T) [axial multipoles (G or M)] when $\chi^{[0 \times 1]}$ is the polar (axial) tensor. The dipoles $X_x, X_y,$ and X_z in Eq. (19) are $X_i = \chi_{0,i}^{[0 \times 1]}$ ($i = x, y, z$).

The response tensor $\chi^{[1 \times 0]}$ is obtained by transposing $\chi^{[0 \times 1]}$, which is expressed by the same type of multipole as $\chi^{[0 \times 1]}$.

The electrocaloric (magnetocaloric) effect where the entropy variation ΔS is induced by the electric field (the magnetic field) as $\Delta S = \sum_i p_i E_i$ ($\Delta S = \sum_i q_i H_i$) is described by one of the rank-1 response tensors. As ΔS corresponds to the E monopole (Q_0), the tensor component of p_i (q_i) is described by the E dipole (Q_x, Q_y, Q_z) or MT dipole (T_x, T_y, T_z) [the ET dipole (G_x, G_y, G_z) or M dipole (M_x, M_y, M_z)]. Here and hereafter in Sec. VA, we do not distinguish the multipoles with the opposite time-reversal parity for simplicity, which depends on the microscopic process in the presence/absence of the dissipation, as discussed in Secs. VB and VC.

2. Rank-2 tensor

We consider two types of rank-2 tensors, $\chi^{[1 \times 1]}$ and $\chi^{[0 \times 2]}$. $\chi^{[1 \times 1]}$ is the response tensor for $B^{[1]} = (B_x, B_y, B_z)$ and $F^{[1]} = (F_x, F_y, F_z)$, which is related with the rank-0 to 2 multipoles as monopole X_0 , dipole (Y_x, Y_y, Y_z), and quadrupole ($X_u, X_v, X_{yz}, X_{zx}, X_{xy}$). The tensor component of $\chi^{[1 \times 1]}$ is given by

$$\chi^{[1 \times 1]} = \begin{pmatrix} X_0 - X_u + X_v & X_{xy} + Y_z & X_{zx} - Y_y \\ X_{xy} - Y_z & X_0 - X_u - X_v & X_{yz} + Y_x \\ X_{zx} + Y_y & X_{yz} - Y_x & X_0 + 2X_u \end{pmatrix}, \quad (20)$$

where $X = Q$ or T (G or M) and $Y = G$ or M (Q or T) for the polar (axial) tensor. See Appendix F 1 for details. When $\chi^{[1 \times 1]}$ is a polar tensor, such as the magnetic susceptibility tensor for $F^{[1]} = \mathbf{H}$ and $B^{[1]} = \mathbf{M}$, the dielectric susceptibility tensor for $F^{[1]} = \mathbf{E}$ and $B^{[1]} = \mathbf{P}$, and the electric conductivity tensor for $F^{[1]} = \mathbf{E}$ and $B^{[1]} = \mathbf{J}$, the corresponding multipoles are the E (MT) monopole and E (MT) quadrupoles for X and ET (M) dipoles for Y . Meanwhile, when $\chi^{[1 \times 1]}$ is an axial tensor, such as the magnetoelectric tensor for $F^{[1]} = \mathbf{E}$ and $B^{[1]} = \mathbf{M}$ or $F^{[1]} = \mathbf{H}$ and $B^{[1]} = \mathbf{P}$, the ET (M) monopole and ET (M) quadrupoles for X and E (MT) dipoles for Y are relevant.

$\chi^{[0 \times 2]}$ is another rank-2 tensor for $B^{[0]} = (B)$ and $F^{[2]} = (F_{xx}, F_{yy}, F_{zz}, F_{yz}, F_{zx}, F_{xy})$, where $F_{ij} = F_{ji}$. As $F^{[2]}$ is decomposed into the monopole and quadrupole components, the tensor component of $\chi^{[0 \times 2]}$ is given by

$$\chi^{[0 \times 2]} = \begin{pmatrix} X_0 - X_u + X_v \\ X_0 - X_u - X_v \\ X_0 + 2X_u \\ X_{yz} \\ X_{zx} \\ X_{xy} \end{pmatrix}^T. \quad (21)$$

Thus the active monopole and quadrupole contribute to $\chi^{[0 \times 2]}$. See Appendix F 2 for details. For example, the piezocaloric tensor for $F^{[2]} = \boldsymbol{\tau}$ and $B^{[0]} = \Delta S$ corresponds to $\chi^{[0 \times 2]}$, where the E (MT) monopole and quadrupole are relevant. The multipole expression of $\chi^{[2 \times 0]}$ is obtained by transposing $\chi^{[0 \times 2]}$.

3. Rank-3 tensor

We consider two types of rank-3 tensors, $\chi^{[1 \times 2]}$ and $\chi^{[0 \times 3]}$. $\chi^{[1 \times 2]}$ is the rank-3 tensor for $B^{[1]} = (B_x, B_y, B_z)$ and $F^{[2]} = (F_{xx}, F_{yy}, F_{zz}, F_{yz}, F_{zx}, F_{xy})$, which is expressed by dipole (X_x, X_y, X_z) , quadrupole $(Y_u, Y_v, Y_{yz}, Y_{zx}, Y_{xy})$, and octupole $(X_{xyz}, X_x^\alpha, X_y^\alpha, X_z^\alpha, X_x^\beta, X_y^\beta, X_z^\beta)$ as

$$\chi^{[1 \times 2]} = \begin{pmatrix} \tilde{X}_x + 4X_x^\alpha & \tilde{X}'_y - 2Y_{zx} - 2X_y^\alpha - 2X_y^\beta & \tilde{X}'_z + 2Y_{xy} - 2X_z^\alpha + 2X_z^\beta \\ \tilde{X}'_x + 2Y_{yz} - 2X_x^\alpha + 2X_x^\beta & \tilde{X}_y + 4X_y^\alpha & \tilde{X}'_z - 2Y_{xy} - 2X_z^\alpha - 2X_z^\beta \\ \tilde{X}'_x - 2Y_{yz} - 2X_x^\alpha - 2X_x^\beta & \tilde{X}'_y + 2Y_{zx} - 2X_y^\alpha + 2X_y^\beta & \tilde{X}_z + 4X_z^\alpha \\ Y_u + Y_v + X_{xyz} & -3X_z + Y_{xy} - 2X_z^\alpha - 2X_z^\beta & -3X_y - Y_{zx} - 2X_y^\alpha + 2X_y^\beta \\ -3X_z - Y_{xy} - 2X_z^\alpha + 2X_z^\beta & -Y_u + Y_v + X_{xyz} & -3X_x + Y_{yz} - 2X_x^\alpha - 2X_x^\beta \\ -3X_y + Y_{zx} - 2X_y^\alpha - 2X_y^\beta & -3X_x - Y_{yz} - 2X_x^\alpha + 2X_x^\beta & -2Y_v + X_{xyz} \end{pmatrix}^T. \quad (22)$$

It is noted that both \tilde{X}_i and \tilde{X}'_i ($i = x, y, z$) stand for the dipole, but they are independent of each other. See Appendix F3 for details. $\chi^{[1 \times 2]}$ is polar for the piezoelectric tensor ($F^{[2]} = \tau, B^{[1]} = \mathbf{P}$) and second-order nonlinear conductivity ($F^{[2]}_{ij} = E_i E_j, B^{[1]} = \mathbf{J}$), where $X = Q$ or T and $Y = G$ or M , while it is axial for the piezomagnetic tensor ($F^{[2]} = \tau, B^{[1]} = \mathbf{M}$), where $X = G$ or M and $Y = Q$ or T . The multipole expression of the tensor $\chi^{[2 \times 1]}$, e.g., the spin conductivity tensor ($F^{[1]} = \mathbf{E}, B^{[2]} = \mathbf{J}^s$), is obtained by transposing the piezomagnetic tensor.

$\chi^{[0 \times 3]}$ is the rank-3 response tensor for $B^{[0]} = (B)$ and $F^{[3]} = (F_{xxx}, F_{yyy}, F_{zzz}, F_{yyz}, F_{zzx}, F_{xxy}, F_{yzz}, F_{zxx}, F_{xyy}, F_{xyz})$, where $F_{ijk} = F_{jik} = F_{ikj}$. As $F^{[3]}$ is decomposed into the dipole and octupole components, $\chi^{[0 \times 3]}$ is also related to them, which is shown as

$$\chi^{[0 \times 3]} = \begin{pmatrix} 3X_x + 2X_x^\alpha \\ 3X_y + 2X_y^\alpha \\ 3X_z + 2X_z^\alpha \\ X_z - X_z^\alpha - X_z^\beta \\ X_x - X_x^\alpha - X_x^\beta \\ X_y - X_y^\alpha - X_y^\beta \\ X_y - X_y^\alpha + X_y^\beta \\ X_z - X_z^\alpha + X_z^\beta \\ X_x - X_x^\alpha + X_x^\beta \\ X_{xyz} \end{pmatrix}^T. \quad (23)$$

See Appendix F4 for details. $\chi^{[0 \times 3]}$, such as the third-order electrocaloric effect, is relevant with $X = Q$ or T (G or M) for the polar (axial) tensor. The multipole expression of $\chi^{[3 \times 0]}$ is obtained by transposing $\chi^{[0 \times 3]}$.

4. Rank-4 tensor

We consider two types of rank-4 tensors, $\chi^{[1 \times 3]}$ and $\chi^{[2 \times 2]}$. $\chi^{[1 \times 3]}$ is the rank-4 response tensor for $B^{[1]} = (B_x, B_y, B_z)$ and $F^{[3]} = (F_{xxx}, F_{yyy}, F_{zzz}, F_{yyz}, F_{zzx}, F_{xxy}, F_{yzz}, F_{zxx}, F_{xyy}, F_{xyz})$, where $F_{ijk} = F_{jik} = F_{ikj}$. The relevant multipoles are from rank 0 to 4: monopole X_0 , dipole (Y_x, Y_y, Y_z) , quadrupole $(X_u, X_v, X_{yz}, X_{zx}, X_{xy})$, octupole $(Y_{xyz}, Y_x^\alpha, Y_y^\alpha, Y_z^\alpha, Y_x^\beta, Y_y^\beta, Y_z^\beta)$, and hexadecapole $(X_4, X_{4u}, X_{4v}, X_{4x}^\alpha, X_{4y}^\alpha, X_{4z}^\alpha, X_{4x}^\beta, X_{4y}^\beta, X_{4z}^\beta)$. The tensor component of $\chi^{[1 \times 3]}$ is given as

$$\chi^{[1 \times 3]} = \begin{pmatrix} 3(X_0 - \tilde{X}_u + \tilde{X}_v) + 2X_4 - X_{4u} + X_{4v} & 3(-Y_z - \tilde{X}_{xy} + Y_z^\alpha - Y_z^\beta) + X_{4z}^\alpha - X_{4z}^\beta & 3(Y_y - \tilde{X}_{zx} - Y_y^\alpha - Y_y^\beta) - X_{4y}^\alpha - X_{4y}^\beta \\ 3(Y_z - \tilde{X}_{xy} - Y_z^\alpha - Y_z^\beta) - X_{4z}^\alpha - X_{4z}^\beta & 3(X_0 - \tilde{X}_u - \tilde{X}_v) + 2X_4 - X_{4u} - X_{4v} & 3(-Y_x - \tilde{X}_{yz} + Y_x^\alpha - Y_x^\beta) + X_{4x}^\alpha - X_{4x}^\beta \\ 3(-Y_y - \tilde{X}_{zx} + Y_y^\alpha - Y_y^\beta) + X_{4y}^\alpha - X_{4y}^\beta & 3(Y_x - \tilde{X}_{yz} - Y_x^\alpha - Y_x^\beta) - X_{4x}^\alpha - X_{4x}^\beta & 3(X_0 + 2\tilde{X}_u) + 2X_4 + 2X_{4u} \\ -Y_y - \tilde{X}_{zx} - 4Y_y^\alpha + 2Y_y^\beta + 2X_{4y}^\beta & Y_x + \tilde{X}'_{yz} - Y_x^\alpha + Y_x^\beta + X_{4x}^\alpha - X_{4x}^\beta & X_0 + \tilde{X}'_u - 5X_v - Y_{xyz} - X_4 - X_{4u} + X_{4v} \\ X_0 + \tilde{X}'_u - \tilde{X}'_v - Y_{xyz} - X_4 - X_{4u} - X_{4v} & -Y_z - \tilde{X}_{xy} - 4Y_z^\alpha + 2Y_z^\beta + 2X_{4z}^\beta & Y_y + \tilde{X}'_v - Y_y^\alpha + Y_y^\beta + X_{4y}^\alpha - X_{4y}^\beta \\ Y_z + \tilde{X}'_{xy} - Y_z^\alpha + Y_z^\beta + X_{4z}^\alpha - X_{4z}^\beta & X_0 - \tilde{X}_u + \tilde{X}'_v - Y_{xyz} - X_4 + 2X_{4u} & -Y_x - \tilde{X}_{yz} - 4Y_x^\alpha + 2Y_x^\beta + 2X_{4x}^\beta \\ Y_z - \tilde{X}_{xy} + 4Y_z^\alpha + 2Y_z^\beta + 2X_{4z}^\beta & X_0 + \tilde{X}'_u + \tilde{X}'_v + Y_{xyz} - X_4 - X_{4u} + X_{4v} & -Y_x + \tilde{X}'_{yz} + Y_x^\alpha + Y_x^\beta - X_{4x}^\alpha - X_{4x}^\beta \\ -Y_y + \tilde{X}'_{zx} + Y_y^\alpha + Y_y^\beta - X_{4y}^\alpha - X_{4y}^\beta & Y_x - \tilde{X}_{yz} + 4Y_x^\alpha + 2Y_x^\beta + 2X_{4x}^\beta & X_0 + \tilde{X}'_u + 5X_v + Y_{yz} - X_4 - X_{4u} - X_{4v} \\ X_0 - \tilde{X}_u - \tilde{X}'_v + Y_{yz} - X_4 + 2X_{4u} & -Y_z + \tilde{X}'_{xy} + Y_z^\alpha + Y_z^\beta - X_{4z}^\alpha - X_{4z}^\beta & Y_y - \tilde{X}_{zx} + 4Y_y^\alpha + 2Y_y^\beta + 2X_{4y}^\beta \\ 5X_{yz} - 2Y_x^\beta + 2X_{4x}^\beta & 5X_{zx} - 2Y_y^\beta + 2X_{4y}^\beta & 5X_{xy} - 2Y_z^\beta + 2X_{4z}^\beta \end{pmatrix}^T. \quad (24)$$

Note that $(\tilde{X}_u, \tilde{X}'_u, \tilde{X}''_u)$, $(\tilde{X}_v, \tilde{X}'_v, \tilde{X}''_v)$, and $(\tilde{X}_{yz}, \tilde{X}'_{yz})$ (cyclic) are introduced to express the two independent quadrupoles. See Appendix F5 for details. $\chi^{[1 \times 3]}$ corresponds to the response tensors, such as the third-order nonlinear electric conductivity. The relevant multipoles are $X = Q$ or T and $Y = G$ or M for the polar tensor, while those are $X = G$ or M and $Y = Q$ or T for the axial tensor. The multipole expression of $\chi^{[3 \times 1]}$ is obtained by transposing $\chi^{[1 \times 3]}$.

$\chi^{[2 \times 2]}$ is another rank-4 tensor for $B^{[2]} = (B_{xx}, B_{yy}, B_{zz}, B_{yz}, B_{zx}, B_{xy})$, where $B_{ij} = B_{ji}$ and $F^{[2]} = (F_{xx}, F_{yy}, F_{zz}, F_{yz}, F_{zx}, F_{xy})$ where $F_{ij} = F_{ji}$. The tensor component of $\chi^{[2 \times 2]}$ is related to the rank 0–4 multipoles, which is given by

$$\chi^{[2 \times 2]} = \begin{pmatrix} \chi_{ll} & \chi_{lt} \\ \chi_{lt} & \chi_{tt} \end{pmatrix}, \quad (25)$$

$$\chi_{ll} = \begin{pmatrix} \tilde{X}_0 + \tilde{X}_u + \tilde{X}_v + 2X_4 - X_{4u} + X_{4v} & \tilde{X}'_0 + \tilde{X}'_u - 2X_v^{(-)} + X_{xyz} - X_4 + 2X_{4u} & \tilde{X}'_0 + \tilde{X}'_u^{(+)} + \tilde{X}'_v^{(-)} - X_{xyz} - X_{4uv+} \\ \tilde{X}'_0 + \tilde{X}'_u + 2X_v^{(-)} - X_{xyz} - X_4 + 2X_{4u} & \tilde{X}_0 + \tilde{X}_u - \tilde{X}_v + 2X_4 - X_{4u} - X_{4v} & \tilde{X}'_0 + \tilde{X}'_u^{(+)} - \tilde{X}'_v^{(-)} + X_{xyz} - X_{4uv-} \\ \tilde{X}'_0 + \tilde{X}'_u^{(+)} + \tilde{X}'_v^{(-)} + X_{xyz} - X_{4uv+} & \tilde{X}'_0 + \tilde{X}'_u^{(-)} - \tilde{X}'_v^{(+)} - X_{xyz} - X_{4uv-} & \tilde{X}_0 - 2\tilde{X}_u + 2X_4 + 2X_{4u} \end{pmatrix}, \quad (26)$$

$$\chi_{lt} = \begin{pmatrix} \tilde{X}_{yz}^{(+)} - 2Y_x^\beta + 2X_{4x}^\beta & -2Y_y + \tilde{X}_{zx}^{(+)} + Y_y^\alpha + Y_y^\beta - X_{4y}^\alpha - X_{4y}^\beta & 2Y_z + \tilde{X}_{xy}^{(+)} - Y_z^\alpha + Y_z^\beta + X_{4z}^\alpha - X_{4z}^\beta \\ 2Y_x + \tilde{X}_{yz}^{(+)} - Y_x^\alpha + Y_x^\beta + X_{4x}^\alpha - X_{4x}^\beta & \tilde{X}_{zx}^{(+)} - 2Y_y^\beta + 2X_{4y}^\beta & -2Y_z + \tilde{X}_{xy}^{(+)} + Y_z^\alpha + Y_z^\beta - X_{4z}^\alpha - X_{4z}^\beta \\ -2Y_x + \tilde{X}_{yz}^{(+)} + Y_x^\alpha + Y_x^\beta - X_{4x}^\alpha - X_{4x}^\beta & 2Y_y + \tilde{X}_{zx}^{(+)} - Y_y^\alpha + Y_y^\beta + X_{4y}^\alpha - X_{4y}^\beta & \tilde{X}_{xy}^{(+)} - 2Y_z^\beta + 2X_{4z}^\beta \end{pmatrix}, \quad (27)$$

$$\chi_{tl} = \begin{pmatrix} \tilde{X}_{yz}^{(-)} + 2Y_x^\beta + 2X_{4x}^\beta & -2Y_x + \tilde{X}_{yz}^{(-)} + Y_x^\alpha - Y_x^\beta + X_{4x}^\alpha - X_{4x}^\beta & 2Y_x + \tilde{X}_{yz}^{(-)} - Y_x^\alpha - Y_x^\beta - X_{4x}^\alpha - X_{4x}^\beta \\ 2Y_y + \tilde{X}_{yz}^{(-)} - Y_y^\alpha - Y_y^\beta - X_{4y}^\alpha - X_{4y}^\beta & \tilde{X}_{zx}^{(-)} + 2Y_y^\beta + 2X_{4y}^\beta & -2Y_y + \tilde{X}_{xy}^{(-)} + Y_y^\alpha - Y_y^\beta + X_{4y}^\alpha - X_{4y}^\beta \\ -2Y_z + \tilde{X}_{xy}^{(-)} + Y_z^\alpha - Y_z^\beta + X_{4z}^\alpha - X_{4z}^\beta & 2Y_z + \tilde{X}_{xy}^{(-)} - Y_z^\alpha - Y_z^\beta - X_{4z}^\alpha - X_{4z}^\beta & \tilde{X}_{xy}^{(-)} + 2Y_z^\beta + 2X_{4z}^\beta \end{pmatrix}, \quad (28)$$

$$\chi_{tt} = \begin{pmatrix} 3X_0 + 3X_u - 3X_v - X_{4uv-} & -Y_z + 3X_{xy} - 2Y_z^\alpha + 2X_{4z}^\beta & Y_y + 3X_{zx} + 2Y_y^\alpha + 2X_{4y}^\beta \\ Y_z + 3X_{xy} + 2Y_z^\alpha + 2X_{4z}^\beta & 3X_0 + 3X_u + 3X_v - X_{4uv+} & -Y_x + 3X_{yz} - 2Y_x^\alpha + 2X_{4x}^\beta \\ -Y_y + 3X_{zx} - 2Y_y^\alpha + 2X_{4y}^\beta & Y_x + 3X_{yz} + 2Y_x^\alpha + 2X_{4x}^\beta & 3X_0 - 6X_u - X_4 + 2X_{4u} \end{pmatrix}, \quad (29)$$

where $X_{4uv\pm} = X_4 + X_{4u} \pm X_{4v}$. We also introduce $(\tilde{X}_0, \tilde{X}'_0)$, $(\tilde{X}_u, \tilde{X}_u^{(\pm)}, \tilde{X}'_u)$, $(\tilde{X}_v, \tilde{X}_v^{(\pm)})$, and $(\tilde{X}_{yz}^{(\pm)}, \tilde{X}'_{yz}^{(\pm)})$ (cyclic) for notational simplicity. See Appendix F6 for details. $\chi^{[2 \times 2]}$ represents the rank-4 tensor, such as the elastic stiffness tensor and magneto-Seebeck tensor, which are related to the multipoles $X = Q$ or T and $Y = G$ or M for the polar tensor and to $X = G$ or M and $Y = Q$ or T for the axial tensor.

B. Linear response theory

The multipoles with the opposite time-reversal parities, E and MT or ET and M, are not distinguished by the above symmetry analyses. They are distinguished from the microscopic process by considering the effect of the dissipation. To demonstrate that, we adopt the Kubo formula in the following discussion [33,70].

When we consider the external perturbation Hamiltonian $\mathcal{H}_{\text{ext}} = -\sum_j \hat{A}_j F_j(t)$, where $F_j(t) = \int_{-\infty}^{\infty} \frac{d\omega}{2\pi} F_{j,\omega} e^{-i\omega t + \delta t}$ is the j th component of an external field for $\delta > 0$, the linear complex susceptibility $\chi_{i;j}(\omega)$ satisfies the relation

$$\langle \hat{B}_{i,\omega} \rangle = \int_{-\infty}^{\infty} \frac{d\omega'}{2\pi} \delta(\omega - \omega') \chi_{i;j}(\omega') F_{j,\omega'}. \quad (30)$$

Considering the uniform external field with the wave vector $\mathbf{q} \rightarrow \mathbf{0}$ and then taking the static limit $\omega \rightarrow 0$, the linear response function for the periodic system is represented as

$$\begin{aligned} \chi_{i;j} &\equiv \chi_{i;j}(\omega \rightarrow 0) \\ &= -\frac{i\hbar}{V} \sum_{knm} \frac{f[\varepsilon_n(\mathbf{k})] - f[\varepsilon_m(\mathbf{k})]}{\varepsilon_n(\mathbf{k}) - \varepsilon_m(\mathbf{k})} \frac{B_{ik}^{nm} \dot{A}_{jk}^{mn}}{i\hbar\delta + \varepsilon_n(\mathbf{k}) - \varepsilon_m(\mathbf{k})}, \end{aligned} \quad (31)$$

where $\dot{A} = dA/dt$. $X_k^{nm} \equiv \langle n\mathbf{k} | \hat{X} | m\mathbf{k} \rangle$ is the matrix element between the Bloch states $|n\mathbf{k}\rangle$ and $|m\mathbf{k}\rangle$ with the band indices n and m , respectively, and the wave vector \mathbf{k} . $f[\varepsilon_n(\mathbf{k})]$ is the Fermi distribution function with the eigenenergy $\varepsilon_n(\mathbf{k})$ of the eigenstate $|n\mathbf{k}\rangle$. V , \hbar , and δ are the system volume, the reduced Planck constant, and the broadening factor, respectively. We here assume the relaxation-time approximation and mimic the constant $1/\delta$ as the relaxation time. $\chi_{i;j}$ can be decomposed as

$$\chi_{i;j} = \chi_{i;j}^{(J)} + \chi_{i;j}^{(E)}, \quad (32)$$

$$\begin{aligned} \chi_{i;j}^{(J)} &= -\frac{\hbar^2 \delta}{V} \sum_{knm} \frac{f[\varepsilon_n(\mathbf{k})] - f[\varepsilon_m(\mathbf{k})]}{\varepsilon_n(\mathbf{k}) - \varepsilon_m(\mathbf{k})} \\ &\quad \times \frac{B_{ik}^{nm} \dot{A}_{jk}^{mn}}{(\hbar\delta)^2 + [\varepsilon_n(\mathbf{k}) - \varepsilon_m(\mathbf{k})]^2}, \end{aligned} \quad (33)$$

$$\chi_{i;j}^{(E)} = -\frac{i\hbar}{V} \sum_{knm}^{\neq} \frac{f[\varepsilon_n(\mathbf{k})] - f[\varepsilon_m(\mathbf{k})]}{(\hbar\delta)^2 + [\varepsilon_n(\mathbf{k}) - \varepsilon_m(\mathbf{k})]^2} B_{ik}^{nm} \dot{A}_{jk}^{mn}, \quad (34)$$

where $\chi_{i;j}^{(J)}$ includes the intraband (dissipative) contribution proportional to $1/\delta$, while $\chi_{i;j}^{(E)}$ is the interband (nondissipative) one, which remains finite in the clean limit of $\delta \rightarrow 0$.

TABLE XIII. Correspondence between the linear response functions $\chi^{(J,E)}$ and multipoles X_{lm} ($l = 1-4$, $X = Q, G, T, M$). Nonzero $\chi^{(J,E)}$ is indicated by the checkmark (\checkmark). In the rightmost column, the parenthesis represents the corresponding multipoles to the response B and the external field F (see also Table XIII).

Rank	$t_{B_i} t_{A_j}$		Multipole	$(\mathcal{P}, \mathcal{T}, \mathcal{PT}) =$				Examples ($B \leftrightarrow F$)		
				$(\bigcirc, \bigcirc, \bigcirc)$	$(\times, \bigcirc, \times)$	$(\bigcirc, \times, \times)$	$(\times, \times, \bigcirc)$		(\times, \times, \times)	
1	Polar	+1	$\chi^{(J)}$ T_{1m}				\checkmark	\checkmark	Electrocaloric tensor ($Q_0 \leftrightarrow Q_{1m}$)	
		$\chi^{(E)}$ Q_{1m}	\checkmark				\checkmark			
	Axial	-1	$\chi^{(J)}$ Q_{1m}		\checkmark			\checkmark	Toroidalcaloric tensor ($Q_0 \leftrightarrow T_{1m}$)	
		$\chi^{(E)}$ T_{1m}				\checkmark	\checkmark			
		+1	$\chi^{(J)}$ M_{1m}			\checkmark		\checkmark		E.g. ($Q_0 \leftrightarrow G_{1m}$)
		$\chi^{(E)}$ G_{1m}	\checkmark	\checkmark	\checkmark	\checkmark	\checkmark			
-1	$\chi^{(J)}$ G_{1m}	\checkmark	\checkmark	\checkmark	\checkmark	\checkmark	Magnetocaloric tensor ($Q_0 \leftrightarrow M_{1m}$)			
$\chi^{(E)}$ M_{1m}			\checkmark		\checkmark					
2	Polar	+1	$\chi^{(J)}$ T_0, M_{1m}, T_{2m}			\checkmark		\checkmark	Magnetic susceptibility tensor ($M_{1m} \leftrightarrow M_{1m}$)	
		$\chi^{(E)}$ Q_0, G_{1m}, Q_{2m}	\checkmark	\checkmark	\checkmark	\checkmark	\checkmark			
	Axial	-1	$\chi^{(J)}$ Q_0, G_{1m}, Q_{2m}	\checkmark	\checkmark	\checkmark	\checkmark	\checkmark	Electric conductivity tensor ($T_{1m} \leftrightarrow E_{1m}$)	
		$\chi^{(E)}$ T_0, M_{1m}, T_{2m}			\checkmark		\checkmark			
		+1	$\chi^{(J)}$ M_0, T_{1m}, M_{2m}			\checkmark		\checkmark		E.g. ($T_{1m} \leftrightarrow M_{1m}$)
		$\chi^{(E)}$ G_0, Q_{1m}, G_{2m}	\checkmark	\checkmark	\checkmark	\checkmark	\checkmark			
-1	$\chi^{(J)}$ G_0, Q_{1m}, G_{2m}	\checkmark	\checkmark	\checkmark	\checkmark	\checkmark	Magnetoelectric tensor ($M_{1m} \leftrightarrow E_{1m}$)			
$\chi^{(E)}$ M_0, T_{1m}, M_{2m}			\checkmark		\checkmark					
3	Polar	+1	$\chi^{(J)}$ T_{1m}, M_{2m}, T_{3m}				\checkmark	\checkmark	Piezoelectric tensor ($Q_{1m} \leftrightarrow Q_0, Q_{2m}$)	
		$\chi^{(E)}$ Q_{1m}, G_{2m}, Q_{3m}	\checkmark	\checkmark			\checkmark			
	Axial	-1	$\chi^{(J)}$ Q_{1m}, G_{2m}, Q_{3m}	\checkmark	\checkmark			\checkmark	E.g., ($T_{1m} \leftrightarrow Q_0, Q_{2m}$) Spin conductivity tensor ($G_0, Q_{1m}, G_{2m} \leftrightarrow Q_{1m}$) Piezomagnetic tensor ($M_{1m} \leftrightarrow Q_0, Q_{2m}$)	
		$\chi^{(E)}$ T_{1m}, M_{2m}, T_{3m}			\checkmark		\checkmark			
		+1	$\chi^{(J)}$ M_{1m}, T_{2m}, M_{3m}			\checkmark		\checkmark		
		$\chi^{(E)}$ G_{1m}, Q_{2m}, G_{3m}	\checkmark	\checkmark	\checkmark	\checkmark	\checkmark			
-1	$\chi^{(J)}$ G_{1m}, Q_{2m}, G_{3m}	\checkmark	\checkmark	\checkmark	\checkmark	\checkmark				
$\chi^{(E)}$ M_{1m}, T_{2m}, M_{3m}			\checkmark		\checkmark					
4	Polar	+1	$\chi^{(J)}$ $T_0, M_{1m}, T_{2m},$ M_{3m}, T_{4m}			\checkmark		\checkmark	Elastic stiffness tensor ($Q_0, Q_{2m} \leftrightarrow Q_0, Q_{2m}$)	
		$\chi^{(E)}$ $Q_0, G_{1m}, Q_{2m},$ G_{3m}, Q_{4m}	\checkmark	\checkmark	\checkmark	\checkmark	\checkmark			
	Axial	-1	$\chi^{(J)}$ $Q_0, G_{1m}, Q_{2m},$ G_{3m}, Q_{4m}	\checkmark	\checkmark	\checkmark	\checkmark	\checkmark	E.g., ($T_0, T_{2m} \leftrightarrow Q_0, Q_{2m}$)	
		$\chi^{(E)}$ $T_0, M_{1m}, T_{2m},$ M_{3m}, T_{4m}			\checkmark		\checkmark			
		+1	$\chi^{(J)}$ $M_0, T_{1m}, M_{2m},$ T_{3m}, M_{4m}			\checkmark		\checkmark		E.g., ($G_0, G_{2m} \leftrightarrow Q_0, Q_{2m}$)
		$\chi^{(E)}$ $G_0, Q_{1m}, G_{2m},$ Q_{3m}, G_{4m}	\checkmark	\checkmark			\checkmark			
-1	$\chi^{(J)}$ $G_0, Q_{1m}, G_{2m},$ Q_{3m}, G_{4m}	\checkmark	\checkmark			\checkmark	E.g., ($M_0, M_{2m} \leftrightarrow Q_0, Q_{2m}$)			
$\chi^{(E)}$ $M_0, T_{1m}, M_{2m},$ T_{3m}, M_{4m}			\checkmark		\checkmark					

$\chi^{(J)}$ and $\chi^{(E)}$ have the opposite time-reversal property [33,70]. When the time-reversal symmetry is preserved, they are transformed as

$$\chi_{i;j}^{(J)} = -t_{B_i} t_{A_j} \chi_{i;j}^{(J)}, \quad \chi_{i;j}^{(E)} = t_{B_i} t_{A_j} \chi_{i;j}^{(E)}, \quad (35)$$

where $X_k^{nm} = t_X X_{-k}^{\bar{n}\bar{m}}$ for $t_X = \pm 1$ ($X = A_j, B_i$). The $\bar{n}\bar{m}$ band stands for the time-reversal partner of the n th band. Equation (35) means that $\chi_{i;j}^{(J)}$ [$\chi_{i;j}^{(E)}$] can be finite when $t_{B_i} t_{A_j} =$

$-1(+1)$. In other words, $\chi_{i;j}^{(J)}$ [$\chi_{i;j}^{(E)}$] becomes nonzero when the M and MT (E and ET) multipoles are active for $t_{B_i} t_{A_j} = +1$, while $\chi_{i;j}^{(J)}$ [$\chi_{i;j}^{(E)}$] becomes nonzero when the E and ET (M and MT) multipoles are active for $t_{B_i} t_{A_j} = -1$. The multipoles contributing to $\chi_{i;j}^{(J)}$ and $\chi_{i;j}^{(E)}$ are summarized in Table XIII. A similar argument holds for the static isothermal susceptibility such as magnetic susceptibility, which is obtained by $\omega \rightarrow 0$ and then $\mathbf{q} \rightarrow \mathbf{0}$ for $\chi_{i;j}(\omega)$ in Eq. (30) in the nondegenerate system [140].

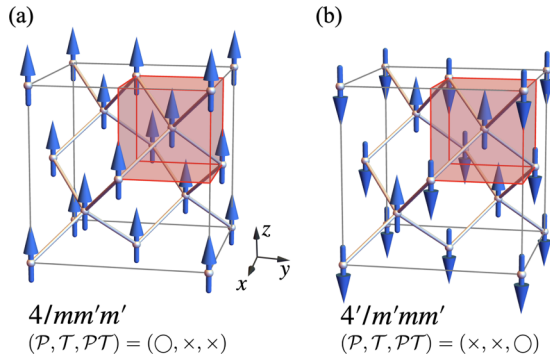


FIG. 2. (a) Ferromagnetic ordering and (b) antiferromagnetic ordering in the diamond structure. (a) is characterized by $4/m\bar{m}m'$ with the \mathcal{P} symmetry, whereas (b) is represented by $4'/m'mm'$ with the \mathcal{PT} symmetry.

Let us discuss $\chi_{ij}^{(J)}$ and $\chi_{ij}^{(E)}$ by taking an example. We consider the uniform and staggered magnetic orderings with magnetic moments along the z axis in the diamond structure in Secs. VB 1 and VB 2, respectively.

1. \mathcal{P} -symmetric magnetic structure

The uniform magnetic structure belonging to the T_{1g}^- representation of $m\bar{3}m1'$ in Fig. 2(a) reduces the symmetry to the \mathcal{P} -symmetric $4/m\bar{m}m'$. From Table IX, one can find that the active multipoles with rank 0–4 are the even-parity E multipoles Q_0 (monopole), Q_u (quadrupole), Q_4 , Q_{4u} (hexadecapole), even-parity M multipoles M_z (dipole), M_z^α (octupole), and even-parity MT multipole T_{4z}^α (hexadecapole). Thus the physical responses related to these active multipoles are expected to occur, such as magnetocaloric response, electric conductivity, and piezomagnetic response from Table XIII.

For example, the electric conductivity tensor $J_i = \sum_j \sigma_{ij} E_j$ is given by

$$\sigma^{(J)} \leftrightarrow \begin{pmatrix} Q_0 - Q_u & 0 & 0 \\ 0 & Q_0 - Q_u & 0 \\ 0 & 0 & Q_0 + 2Q_u \end{pmatrix} \quad (36)$$

and

$$\sigma^{(E)} \leftrightarrow \begin{pmatrix} 0 & M_z & 0 \\ -M_z & 0 & 0 \\ 0 & 0 & 0 \end{pmatrix}, \quad (37)$$

where $\sigma_{ij} = \sigma_{ij}^{(J)} + \sigma_{ij}^{(E)}$. This means that the system exhibits the anisotropic electric conductivity along the xy and z directions and the anomalous Hall effect in the xy plane.

The other example is the piezomagnetic effect where $M_i = \sum_{jk} \Lambda_{ijk} \tau_{jk}$. From the active multipoles, the tensor component is given by

$$\Lambda^{(E)} = \begin{pmatrix} 0 & 0 & \Lambda_{zxx}^{(E)} \\ 0 & 0 & \Lambda_{zxx}^{(E)} \\ 0 & 0 & \Lambda_{zzz}^{(E)} \\ 0 & \Lambda_{yyz}^{(E)} & 0 \\ \Lambda_{yyz}^{(E)} & 0 & 0 \\ 0 & 0 & 0 \end{pmatrix}^T \quad (38)$$

$$\leftrightarrow \begin{pmatrix} 0 & 0 & \tilde{M}'_z - 2M_z^\alpha \\ 0 & 0 & \tilde{M}'_z - 2M_z^\alpha \\ 0 & 0 & \tilde{M}'_z + 4M_z^\alpha \\ 0 & -3M_z - 2M_z^\alpha & 0 \\ -3M_z - 2M_z^\alpha & 0 & 0 \\ 0 & 0 & 0 \end{pmatrix}^T, \quad (39)$$

by using Eq. (22). We omit $\Lambda^{(J)}$ by taking $\delta \rightarrow 0$.

2. \mathcal{PT} -symmetric magnetic structure

The staggered magnetic structure belonging to the T_{2u}^- representation in Fig. 2(b) has the \mathcal{PT} -symmetric $4'/m'mm'$. In this case, the odd-parity M multipoles M_{xy} (quadrupole), M_{4z}^β (hexadecapole), and odd-parity MT multipole T_z^β (octupole) become active in addition to the even-parity E multipoles Q_0 , Q_u , Q_4 , and Q_{4u} , which are obtained by appropriately replacing the mirror plane of $4'/m'mm'$ in Table X. The active odd-parity M and MT multipoles induce the cross-correlated responses such as magnetoelectric effect and piezoelectric effect in Table XIII.

For example, the magnetoelectric tensor α_{ij} is given by

$$\alpha^{(E)} = \begin{pmatrix} 0 & \alpha_{xy}^{(E)} & 0 \\ \alpha_{xy}^{(E)} & 0 & 0 \\ 0 & 0 & 0 \end{pmatrix} \leftrightarrow \begin{pmatrix} 0 & M_{xy} & 0 \\ M_{xy} & 0 & 0 \\ 0 & 0 & 0 \end{pmatrix}. \quad (40)$$

It is noted that $\alpha^{(J)} = 0$, as no odd-parity E and ET multipoles are active under the magnetic point group $4'/m'mm'$.

Meanwhile, in the (inverse) piezoelectric response, the response tensor d_{ijk} for $\varepsilon_{ij} = \sum_k d_{ijk} E_k$ [70,71] is described by M_{xy} and T_z^β as

$$d^{(J)} = \begin{pmatrix} 0 & 0 & d_{xxx} \\ 0 & 0 & -d_{xxx} \\ 0 & 0 & 0 \\ 0 & d_{yzy} & 0 \\ -d_{yzy} & 0 & 0 \\ 0 & 0 & 0 \end{pmatrix} \leftrightarrow \begin{pmatrix} 0 & 0 & -2M_{xy} + 2T_z^\beta \\ 0 & 0 & 2M_{xy} - 2T_z^\beta \\ 0 & 0 & 0 \\ 0 & -M_{xy} - 2T_z^\beta & 0 \\ M_{xy} + 2T_z^\beta & 0 & 0 \\ 0 & 0 & 0 \end{pmatrix}. \quad (41)$$

Similar to α_{ij} , $d_{ijk}^{(E)} = 0$ owing to the lack of odd-parity E and ET multipoles.

C. Nonlinear response theory

In a similar way to the linear response tensor χ_{ij} , we consider the second-order nonlinear response tensor $\chi_{i,jk}$ based on the Kubo formula [141].

The nonlinear complex susceptibility $\chi_{i,jk}(\omega', \omega'')$ satisfies the relation

$$\langle \hat{B}_{i,\omega} \rangle = \int_{-\infty}^{\infty} \int_{-\infty}^{\infty} \frac{d\omega'}{2\pi} \frac{d\omega''}{2\pi} \chi_{i,jk}(\omega', \omega'') F_{j,\omega'} F_{k,\omega''} \delta(\omega - \omega' - \omega''), \quad (42)$$

where $\chi_{i,jk}(\omega', \omega'')$ is represented as

$$\chi_{i,jk}(\omega', \omega'') = \frac{1}{2} \left(\frac{1}{i\hbar} \right)^2 \int_0^{\infty} \int_0^{\infty} dt' dt'' \text{Tr}[\hat{B}_i[\hat{A}_j(-t'), [\hat{A}_k(-t' - t''), \rho_0]]] e^{i(\omega' + \omega'')t' - 2\delta t'} e^{i\omega' t'' - \delta t''} + (j, \omega') \leftrightarrow (k, \omega''), \quad (43)$$

where $\hat{X}(t)$ is the Heisenberg representation of an operator \hat{X} . ρ_0 is the density matrix for the nonperturbative state, whose matrix element is represented by the Fermi distribution function $f(\varepsilon_n)$ as $[\rho_0]_{nm} = f(\varepsilon_n)\delta_{nm}$. When we suppose \hat{A} as the well-defined operator in a periodic system, i.e., the matrix element of \hat{A} includes no differential operator with respect to the wave vector, the nonlinear response function in the static limit ($\mathbf{q} \rightarrow \mathbf{0}$, $\omega \rightarrow 0$) is given as follows:

$$\chi_{i,jk} \equiv \chi_{i,jk}(0, 0) = \frac{1}{2} \frac{1}{V} \sum_{\mathbf{k}} \sum_{lmn} \frac{B_{ik}^{nm} (A_{jk}^{ml} A_{kk}^{ln} + A_{kk}^{ml} A_{jk}^{ln})}{\varepsilon_n(\mathbf{k}) - \varepsilon_m(\mathbf{k}) + 2i\hbar\delta} \left\{ \frac{f[\varepsilon_n(\mathbf{k})] - f[\varepsilon_l(\mathbf{k})]}{\varepsilon_n(\mathbf{k}) - \varepsilon_l(\mathbf{k}) + i\hbar\delta} - \frac{f[\varepsilon_l(\mathbf{k})] - f[\varepsilon_m(\mathbf{k})]}{\varepsilon_l(\mathbf{k}) - \varepsilon_m(\mathbf{k}) + i\hbar\delta} \right\}. \quad (44)$$

The nonlinear response function is also decomposed into the two parts with different time-reversal properties as

$$\chi_{i,jk} = \chi_{i,jk}^{(\text{Re})} + \chi_{i,jk}^{(\text{Im})}, \quad (45)$$

where

$$\begin{aligned} \chi_{i,jk}^{(\text{Re})} \equiv & \frac{1}{V} \sum_{klmn} \frac{\text{Re}(B_{ik}^{nm} A_{jk}^{ml} A_{kk}^{ln}) [\varepsilon_n(\mathbf{k}) - \varepsilon_m(\mathbf{k})]}{[\varepsilon_n(\mathbf{k}) - \varepsilon_m(\mathbf{k})]^2 + (2\hbar\delta)^2} \left(\frac{\{f[\varepsilon_n(\mathbf{k})] - f[\varepsilon_l(\mathbf{k})]\} [\varepsilon_n(\mathbf{k}) - \varepsilon_l(\mathbf{k})]}{[\varepsilon_n(\mathbf{k}) - \varepsilon_l(\mathbf{k})]^2 + (\hbar\delta)^2} \right. \\ & \left. - \frac{\{f[\varepsilon_l(\mathbf{k})] - f[\varepsilon_m(\mathbf{k})]\} [\varepsilon_l(\mathbf{k}) - \varepsilon_m(\mathbf{k})]}{[\varepsilon_l(\mathbf{k}) - \varepsilon_m(\mathbf{k})]^2 + (\hbar\delta)^2} \right) - \frac{2\hbar^2\delta^2}{V} \sum_{klmn} \frac{\text{Re}(B_{ik}^{nm} A_{jk}^{ml} A_{kk}^{ln})}{[\varepsilon_n(\mathbf{k}) - \varepsilon_m(\mathbf{k})]^2 + (2\hbar\delta)^2} \\ & \times \left\{ \frac{f[\varepsilon_n(\mathbf{k})] - f[\varepsilon_l(\mathbf{k})]}{[\varepsilon_n(\mathbf{k}) - \varepsilon_l(\mathbf{k})]^2 + (\hbar\delta)^2} - \frac{f[\varepsilon_l(\mathbf{k})] - f[\varepsilon_m(\mathbf{k})]}{[\varepsilon_l(\mathbf{k}) - \varepsilon_m(\mathbf{k})]^2 + (\hbar\delta)^2} \right\}, \quad (46) \end{aligned}$$

$$\begin{aligned} \chi_{i,jk}^{(\text{Im})} \equiv & \frac{\hbar\delta}{V} \sum_{klmn} \frac{\text{Im}(B_{ik}^{nm} A_{jk}^{ml} A_{kk}^{ln}) [\varepsilon_n(\mathbf{k}) - \varepsilon_m(\mathbf{k})]}{[\varepsilon_n(\mathbf{k}) - \varepsilon_m(\mathbf{k})]^2 + (2\hbar\delta)^2} \left\{ \frac{f[\varepsilon_n(\mathbf{k})] - f[\varepsilon_l(\mathbf{k})]}{[\varepsilon_n(\mathbf{k}) - \varepsilon_l(\mathbf{k})]^2 + (\hbar\delta)^2} - \frac{f[\varepsilon_l(\mathbf{k})] - f[\varepsilon_m(\mathbf{k})]}{[\varepsilon_l(\mathbf{k}) - \varepsilon_m(\mathbf{k})]^2 + (\hbar\delta)^2} \right\} \\ & + \frac{2\hbar\delta}{V} \sum_{klmn} \frac{\text{Im}(B_{ik}^{nm} A_{jk}^{ml} A_{kk}^{ln})}{[\varepsilon_n(\mathbf{k}) - \varepsilon_m(\mathbf{k})]^2 + (2\hbar\delta)^2} \left(\frac{\{f[\varepsilon_n(\mathbf{k})] - f[\varepsilon_l(\mathbf{k})]\} [\varepsilon_n(\mathbf{k}) - \varepsilon_l(\mathbf{k})]}{[\varepsilon_n(\mathbf{k}) - \varepsilon_l(\mathbf{k})]^2 + (\hbar\delta)^2} - \frac{\{f[\varepsilon_l(\mathbf{k})] - f[\varepsilon_m(\mathbf{k})]\} [\varepsilon_l(\mathbf{k}) - \varepsilon_m(\mathbf{k})]}{[\varepsilon_l(\mathbf{k}) - \varepsilon_m(\mathbf{k})]^2 + (\hbar\delta)^2} \right). \quad (47) \end{aligned}$$

In contrast to the linear response tensor χ_{ij} , there are complicated intraband and interband processes in both $\chi_{i,jk}^{(\text{Re})}$ and $\chi_{i,jk}^{(\text{Im})}$. It is noted that the nonlinear response function of electric field in the length gauge needs rederivation by applying $\hat{A} = -e\hat{r}$ (\hat{r} : position operator) in Eq. (43), since the matrix element of \hat{r} in a periodic system includes differential operator of \mathbf{k} [142].

$\chi_{i,jk}^{(\text{Re})}$ and $\chi_{i,jk}^{(\text{Im})}$ show the following relations in the presence of time-reversal symmetry:

$$\chi_{i,jk}^{(\text{Re})} = t_{B_i} t_{A_j} t_{A_k} \chi_{i,jk}^{(\text{Re})}, \quad \chi_{i,jk}^{(\text{Im})} = -t_{B_i} t_{A_j} t_{A_k} \chi_{i,jk}^{(\text{Im})}. \quad (48)$$

Equation (48) indicates that $\chi_{i,jk}^{(\text{Re})}$ and $\chi_{i,jk}^{(\text{Im})}$ are represented by E and ET (M and MT) multipoles and the M and MT (E and ET) multipoles, respectively, for $t_{B_i} t_{A_j} t_{A_k} = +1(-1)$. The multipoles relevant with the nonlinear response tensors are shown in Table XIV. In the following we show a correspondence between the nonlinear responses and multipoles by considering again the ferromagnetic and AFM orderings in the diamond structure in Figs. 2(a) and 2(b).

1. \mathcal{P} -symmetric magnetic structure

In the \mathcal{P} -symmetric ferromagnetic structure in Fig. 2(a), the nonlinear responses, such as the Nernst effect and the

TABLE XIV. Correspondence between the second-order nonlinear response functions $\chi^{(\text{Re,Im})}$ and multipoles. Nonzero $\chi^{(\text{Re,Im})}$ is shown by the checkmark (\checkmark).

Rank	$t_{B_i} t_{A_j} t_{A_k}$	Multipole	$(\mathcal{P}, \mathcal{T}, \mathcal{PT}) =$					Examples ($B \leftrightarrow F$)		
			$(\bigcirc, \bigcirc, \bigcirc)$	$(\times, \bigcirc, \times)$	$(\bigcirc, \times, \times)$	$(\times, \times, \bigcirc)$	(\times, \times, \times)			
3	Polar	+1	$\chi^{(\text{Im})}$ T_{1m}, M_{2m}, T_{3m}				\checkmark	\checkmark	E.g., ($Q_{1m} \leftrightarrow Q_0, Q_{2m}$) Electric conductivity tensor ($T_{1m} \leftrightarrow Q_0, Q_{2m}$) Nernst effect tensor ($T_{1m} \leftrightarrow M_0, M_{2m}$) Magnetoelectric tensor ($M_{1m} \leftrightarrow Q_0, Q_{2m}$)	
		$\chi^{(\text{Re})}$ Q_{1m}, G_{2m}, Q_{3m}	\checkmark				\checkmark			
	-1	$\chi^{(\text{Im})}$ Q_{1m}, G_{2m}, Q_{3m}		\checkmark			\checkmark			
	$\chi^{(\text{Re})}$ T_{1m}, M_{2m}, T_{3m}				\checkmark	\checkmark				
	Axial	+1	$\chi^{(\text{Im})}$ M_{1m}, T_{2m}, M_{3m}			\checkmark		\checkmark		
		$\chi^{(\text{Re})}$ G_{1m}, Q_{2m}, G_{3m}	\checkmark	\checkmark	\checkmark	\checkmark	\checkmark			
	-1	$\chi^{(\text{Im})}$ G_{1m}, Q_{2m}, G_{3m}	\checkmark	\checkmark	\checkmark	\checkmark	\checkmark			
	$\chi^{(\text{Re})}$ M_{1m}, T_{2m}, M_{3m}				\checkmark	\checkmark				
4	Polar	+1	$\chi^{(\text{Im})}$ $T_0, M_{1m}, T_{2m},$ M_{3m}, T_{4m}			\checkmark		\checkmark	Electric striction tensor ($Q_0, Q_{2m} \leftrightarrow Q_0, Q_{2m}$)	
		$\chi^{(\text{Re})}$ $Q_0, G_{1m}, Q_{2m},$ G_{3m}, Q_{4m}	\checkmark	\checkmark	\checkmark	\checkmark	\checkmark			
		-1	$\chi^{(\text{Im})}$ $Q_0, G_{1m}, Q_{2m},$ G_{3m}, Q_{4m}	\checkmark	\checkmark	\checkmark	\checkmark	\checkmark		E.g., ($Q_0, Q_{2m} \leftrightarrow T_0, T_{2m}$)
		$\chi^{(\text{Re})}$ $T_0, M_{1m}, T_{2m},$ M_{3m}, T_{4m}			\checkmark		\checkmark			
	Axial	+1	$\chi^{(\text{Im})}$ $M_0, T_{1m}, M_{2m},$ T_{3m}, M_{4m}				\checkmark	\checkmark	E.g., ($Q_0, Q_{2m} \leftrightarrow G_0, G_{2m}$)	
		$\chi^{(\text{Re})}$ $G_0, Q_{1m}, G_{2m},$ Q_{3m}, G_{4m}		\checkmark			\checkmark			
		-1	$\chi^{(\text{Im})}$ $G_0, Q_{1m}, G_{2m},$ Q_{3m}, G_{4m}		\checkmark			\checkmark		E.g., ($Q_0, Q_{2m} \leftrightarrow M_0, M_{2m}$)
		$\chi^{(\text{Re})}$ $M_0, T_{1m}, M_{2m},$ T_{3m}, M_{4m}				\checkmark	\checkmark			

second-order nonlinear magnetoelectric effect, are expected. In the case of the nonlinear magnetoelectric effect $M_i = \sum_{jk} \alpha_{ijk} E_j E_k$, the tensor $\alpha_{ijk}^{(\text{Re})}$ is induced by the even-parity M and MT multipoles in Table XIV. Since M_z and M_z^α are active in the $4/m\bar{m}'m'$ symmetry, the tensor component of $\alpha_{ijk}^{(\text{Re})}$ is represented by

$$\alpha^{(\text{Re})} = \begin{pmatrix} 0 & 0 & \alpha_{zxx}^{(\text{E})} \\ 0 & 0 & \alpha_{zxx}^{(\text{E})} \\ 0 & 0 & \alpha_{zzz}^{(\text{E})} \\ 0 & \alpha_{yyz}^{(\text{E})} & 0 \\ \alpha_{yyz}^{(\text{E})} & 0 & 0 \\ 0 & 0 & 0 \end{pmatrix}^T$$

$$\Leftrightarrow \begin{pmatrix} 0 & 0 & \tilde{M}'_z - 2M_z^\alpha \\ 0 & 0 & \tilde{M}'_z - 2M_z^\alpha \\ 0 & 0 & \tilde{M}'_z + 4M_z^\alpha \\ 0 & -3M_z - 2M_z^\alpha & 0 \\ -3M_z - 2M_z^\alpha & 0 & 0 \\ 0 & 0 & 0 \end{pmatrix}^T, \quad (49)$$

where there are three independent matrix elements in $\alpha^{(\text{Re})}$.

2. \mathcal{PT} -symmetric magnetic structure

In the AFM ordering with the $4'/m'mm'$ symmetry in Fig. 2(b), the second-order nonlinear conductivity, σ_{ijk} , for $J_i = \sum_{jk} \sigma_{ijk} E_j E_k$ becomes nonzero, which reflects the lack of the spatial-inversion symmetry. Among the two parts $\sigma_{ijk}^{(\text{Re})}$ and $\sigma_{ijk}^{(\text{Im})}$, $\sigma_{ijk}^{(\text{Re})}$ is induced in the presence of the odd-parity M and MT multipoles. The finite tensor component of $\sigma_{ijk}^{(\text{Re})}$ is shown as

$$\sigma^{(\text{Re})} = \begin{pmatrix} 0 & 0 & \sigma_{xxx}^{(\text{Re})} \\ 0 & 0 & -\sigma_{xxx}^{(\text{Re})} \\ 0 & 0 & 0 \\ 0 & \sigma_{yzy}^{(\text{Re})} & 0 \\ -\sigma_{yzy}^{(\text{Re})} & 0 & 0 \\ 0 & 0 & 0 \end{pmatrix}^T$$

$$\leftrightarrow \begin{pmatrix} 0 & 0 & -2M_{xy} + 2T_z^\beta \\ 0 & 0 & 2M_{xy} - 2T_z^\beta \\ 0 & 0 & 0 \\ 0 & -M_{xy} - 2T_z^\beta & 0 \\ M_{xy} + 2T_z^\beta & 0 & 0 \\ 0 & 0 & 0 \end{pmatrix}^T. \quad (50)$$

Thus the nonlinear conductivity, which is known as the nonlinear Drude and/or the intrinsic terms, is expected in the AFM structure in Fig. 2(b) [143].

VI. SUMMARY

In summary, we have accomplished the classification of the multipole degrees of freedom in accordance with the irreducible (co)representations in 122 magnetic point groups. The completed multipole classification enables us to explore further functional multiferroic materials showing the extraordinary cross-correlated phenomena with exotic ordered states more than ordinary ferromagnetic and AFM orderings. Our multipole classification has mainly three advantages. One is the systematic identification of electronic order parameters to cover unconventional nematic, chiral, excitonic, loop-current, and anisotropic bond ordered states. The second is the predictability of overlooked physical phenomena under simple ferromagnetic and AFM orderings which may be hosted by the secondary multipole order parameters. The third is the intuitive understanding of the multiferroic phenomena and nonlinear transports on the basis of the microscopic multipole couplings. The present comprehensive study will give an efficient way to explore further exotic physical phenomena induced by higher-rank multipoles, e.g., MT quadrupole

and octupole. Moreover, our result can be applied to investigate the functional magnetic materials in cooperation with material databases such as MAGNDATA [144], as the multipole analysis is perfectly compatible with group theoretical analysis.

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APPENDIX A: MULTIPOLE NOTATION UNDER CUBIC AND HEXAGONAL POINT GROUPS

In the main text we adopt the real expressions of $O_{lm}(\mathbf{r})$ for both atomic multipoles in Eqs. (1)–(4) and cluster multipoles in Eqs. (9) and (10), which are given by [90]

$$O_{l0}^{(c)}(\mathbf{r}) \equiv O_{l0}(\mathbf{r}), \quad (A1)$$

$$O_{lm}^{(c)}(\mathbf{r}) \equiv \frac{(-1)^m}{\sqrt{2}} [O_{lm}(\mathbf{r}) + O_{lm}^*(\mathbf{r})], \quad (A2)$$

$$O_{lm}^{(s)}(\mathbf{r}) \equiv i \frac{(-1)^m}{\sqrt{2}} [O_{lm}(\mathbf{r}) - O_{lm}^*(\mathbf{r})]. \quad (A3)$$

A linear combination of $O_{lm}^{(c)}(\mathbf{r})$ and $O_{lm}^{(s)}(\mathbf{r})$ gives the expression of multipoles under the magnetic point groups. In the case of the cubic and its subgroups, the cubic harmonics are used. We show the cubic expressions of $O_{lm}(\mathbf{r})$ up to rank 4 as follows: the rank 0 is

$$O_0 = 1, \quad (A4)$$

TABLE XV. List of 58 black-and-white point groups $M^{(III)}$. The parentheses represent the corresponding unitary subgroup H .

Cubic	Tetragonal	Orthorhombic	Monoclinic	Triclinic	Hexagonal	Trigonal
$m'\bar{3}'m'$ (432)	$4/m'm'm'$ (422)	$m'm'm'$ (222)	$2'/m'$ ($\bar{1}$)	$\bar{1}'$ (1)	$6/m'm'm'$ (622)	$\bar{3}m'$ ($\bar{3}$)
$m\bar{3}m'$ ($m\bar{3}$)	$4/m\bar{m}'m'$ (4/m)	$m'm'm$ (2/m)	$2/m'$ (2)		$6/m\bar{m}'m'$ (6/m)	$\bar{3}'m'$ (32)
$m'\bar{3}'m$ ($\bar{4}3m$)	$4'/m'm'm$ ($\bar{4}2m$)	$m'mm$ (2mm)	$2'/m$ (m)		$6'/n'mm'$ ($\bar{3}m$)	$\bar{3}'m$ (3m)
$\bar{4}'3m'$ (23)	$4'/m\bar{m}'m$ (mmm)	$2'2'2$ (2)	m' (1)		$6'/m\bar{m}'m'$ ($\bar{6}m2$)	$32'$ (3)
$4'32'$ (23)	$4/m'mm$ (4mm)	$m'm'2$ (2)	$2'$ (1)		$6/m'mm$ (6mm)	$3m'$ (3)
$m'\bar{3}'$ (23)	$42'2'$ (4)	$m'm2'$ (m)			$62'2'$ (6)	$\bar{3}'$ (3)
	$4'22'$ (222)				$6'22'$ (32)	
	$\bar{4}2'm'$ ($\bar{4}$)				$\bar{6}m'2'$ ($\bar{6}$)	
	$\bar{4}'2m'$ (222)				$\bar{6}'m2'$ (3m)	
	$\bar{4}'2'm$ (mm2)				$\bar{6}'m'2$ (32)	
	$4m'm'$ (4)				$6m'm'$ (6)	
	$4'm'm$ (mm2)				$6'mm'$ (3m)	
	$4'/m'$ ($\bar{4}$)				$6'/m'$ ($\bar{3}$)	
	$4/m'$ (4)				$6/m'$ (6)	
	$4'/m$ (2/m)				$6'/m$ ($\bar{6}$)	
	$\bar{4}'$ (2)				$\bar{6}'$ (3)	
	$4'$ (2)				$6'$ (3)	

TABLE XVI. Primary, secondary, and tertiary axes with respect to the symmetry operations in the Cartesian coordinates.

	Primary	Secondary	Tertiary
Cubic	$\langle 100 \rangle$	$\langle 111 \rangle$	$\langle 110 \rangle$
Tetragonal	$[001]$	$[100]$	$[110]$
Orthorhombic	$[100]$	$[010]$	$[001]$
Monoclinic	$[010]$		
Triclinic			
Hexagonal	$[001]$	$[100]$	$[010]$
Trigonal	$[001]$	$[010]$	

the rank 1 is

$$(O_x, O_y, O_z) = (x, y, z), \quad (\text{A5})$$

the rank 2 is

$$O_u = \frac{1}{2}(3z^2 - r^2), \quad (\text{A6})$$

$$O_v = \frac{\sqrt{3}}{2}(x^2 - y^2), \quad (\text{A7})$$

$$(O_{yz}, O_{zx}, O_{xy}) = \sqrt{3}(yz, zx, xy), \quad (\text{A8})$$

the rank 3 is

$$O_{xyz} = \sqrt{15}xyz, \quad (\text{A9})$$

$$(O_x^\alpha, O_y^\alpha, O_z^\alpha) = \frac{1}{2}(x(5x^2 - 3r^2), y(5y^2 - 3r^2), z(5z^2 - 3r^2)), \quad (\text{A10})$$

$$(O_x^\beta, O_y^\beta, O_z^\beta) = \frac{\sqrt{15}}{2}(x(y^2 - z^2), y(z^2 - x^2), z(x^2 - y^2)), \quad (\text{A11})$$

and the rank 4 is

$$O_4 = \frac{5\sqrt{21}}{12}\left(x^4 + y^4 + z^4 - \frac{3}{5}r^4\right), \quad (\text{A12})$$

$$O_{4u} = \frac{7\sqrt{15}}{6}\left[z^4 - \frac{x^4 + y^4}{2} - \frac{3}{7}r^2(3z^2 - r^2)\right], \quad (\text{A13})$$

$$O_{4v} = \frac{7\sqrt{5}}{4}\left[x^4 - y^4 - \frac{6}{7}r^2(x^2 - y^2)\right], \quad (\text{A14})$$

$$(O_{4x}^\alpha, O_{4y}^\alpha, O_{4z}^\alpha) = \frac{\sqrt{35}}{2}(yz(y^2 - z^2), zx(z^2 - x^2), xy(x^2 - y^2)), \quad (\text{A15})$$

$$(O_{4x}^\beta, O_{4y}^\beta, O_{4z}^\beta) = \frac{\sqrt{5}}{2}(yz(7x^2 - r^2), zx(7y^2 - r^2), xy(7z^2 - r^2)), \quad (\text{A16})$$

where we denote $O_{lm}(\mathbf{r}) \rightarrow O_{lm}$ for notation simplicity. In the case of the hexagonal and trigonal point groups, it is useful to

TABLE XVII. IRREPs of magnetic (M) and magnetic toroidal (MT) multipoles ($l \leq 4$) in the cubic gray point groups. The classification for $m\bar{3}m1'$ is shown in Table II.

4321'				
IRREP	MT	M	MPG	P. axis
A_1^-	T_0, T_4	M_0, M_4	432	$\langle 100 \rangle$
A_2^-	T_{xyz}	M_{xyz}	4'32'	$\langle 100 \rangle$
E^-	T_u, T_{4u}	M_u, M_{4u}	422	[001]
	T_v, T_{4v}	M_v, M_{4v}	4'22'	[001]
T_1^-	$T_x, T_x^\alpha, T_{4x}^\alpha$	$M_x, M_x^\alpha, M_{4x}^\alpha$	42'2'	[100]
	$T_y, T_y^\alpha, T_{4y}^\alpha$	$M_y, M_y^\alpha, M_{4y}^\alpha$	42'2'	[010]
	$T_z, T_z^\alpha, T_{4z}^\alpha$	$M_z, M_z^\alpha, M_{4z}^\alpha$	42'2'	[001]
T_2^-	$T_{yz}, T_x^\beta, T_{4x}^\beta$	$M_{yz}, M_x^\beta, M_{4x}^\beta$	4'2'2	[100]
	$T_{zx}, T_y^\beta, T_{4y}^\beta$	$M_{zx}, M_y^\beta, M_{4y}^\beta$	4'2'2	[010]
	$T_{xy}, T_z^\beta, T_{4z}^\beta$	$M_{xy}, M_z^\beta, M_{4z}^\beta$	4'2'2	[001]
$\bar{4}3m1'$				
IRREP	MT	M	MPG	P. axis
A_1^-	T_0, T_{xyz}, T_4		$\bar{4}3m$	$\langle 100 \rangle$
A_2^-		M_0, M_{xyz}, M_4	$\bar{4}'3m'$	$\langle 100 \rangle$
E^-	T_u, T_{4u}	M_v, M_{4v}	$\bar{4}2m$	[001]
	T_v, T_{4v}	M_u, M_{4u}	$\bar{4}'2m'$	[001]
T_1^-	T_x^β, T_{4x}^α	$M_x, M_{yz}, M_x^\alpha, M_{4x}^\beta$	$\bar{4}2'm'$	[100]
	T_y^β, T_{4y}^α	$M_y, M_{zx}, M_y^\alpha, M_{4y}^\beta$	$\bar{4}2'm'$	[010]
	T_z^β, T_{4z}^α	$M_z, M_{xy}, M_z^\alpha, M_{4z}^\beta$	$\bar{4}2'm'$	[001]
T_2^-	$T_x, T_{yz}, T_x^\alpha, T_{4x}^\beta$	M_x^β, M_{4x}^α	$\bar{4}'2'm$	[100]
	$T_y, T_{zx}, T_y^\alpha, T_{4y}^\beta$	M_y^β, M_{4y}^α	$\bar{4}'2'm$	[010]
	$T_z, T_{xy}, T_z^\alpha, T_{4z}^\beta$	M_z^β, M_{4z}^α	$\bar{4}'2'm$	[001]
$m\bar{3}1'$				
IRREP	MT	M	MPG	P. axis
A_g^-	T_0, T_4	M_{xyz}	$m\bar{3}$	$\langle 100 \rangle$
E_g	T_u, T_{4u}		mmm	[100]
	T_v, T_{4v}		mmm	[100]
T_g^-	$T_{yz}, T_{4x}^\alpha, T_{4x}^\beta$	$M_x, M_x^\alpha, M_x^\beta$	$mm'm'$	[100]
	$T_{zx}, T_{4y}^\alpha, T_{4y}^\beta$	$M_y, M_y^\alpha, M_y^\beta$	$m'mm'$	[100]
	$T_{xy}, T_{4z}^\alpha, T_{4z}^\beta$	$M_z, M_z^\alpha, M_z^\beta$	$m'm'm$	[100]
A_u^-	T_{xyz}	M_0, M_4	$m'\bar{3}'$	$\langle 100 \rangle$
E_u		M_u, M_{4u}	$m'm'm'$	[100]
		M_v, M_{4v}	$m'm'm'$	[100]
T_u^-	$T_x, T_x^\alpha, T_x^\beta$	$M_{yz}, M_{4x}^\alpha, M_{4x}^\beta$	$m'mm$	[100]
	$T_y, T_y^\alpha, T_y^\beta$	$M_{zx}, M_{4y}^\alpha, M_{4y}^\beta$	$mm'm$	[100]
	$T_z, T_z^\alpha, T_z^\beta$	$M_{xy}, M_{4z}^\alpha, M_{4z}^\beta$	mmm'	[100]
231'				
IRREP	MT	M	MPG	P. axis
A^-	T_0, T_{xyz}, T_4	M_0, M_{xyz}, M_4	23	$\langle 100 \rangle$
E	T_u, T_{4u}	M_u, M_{4u}	222	[100]
	T_v, T_{4v}	M_v, M_{4v}	222	[100]
T^-	$T_x, T_{yz}, T_x^\alpha, T_x^\beta$	$M_x, M_{yz}, M_x^\alpha, M_x^\beta$	22'2'	[100]
	$T_{4x}^\alpha, T_{4x}^\beta$	$M_{4x}^\alpha, M_{4x}^\beta$		
	$T_y, T_{zx}, T_y^\alpha, T_y^\beta$	$M_y, M_{zx}, M_y^\alpha, M_y^\beta$	2'22'	[100]
	$T_{4y}^\alpha, T_{4y}^\beta$	$M_{4y}^\alpha, M_{4y}^\beta$		
	$T_z, T_{xy}, T_z^\alpha, T_z^\beta$	$M_z, M_{xy}, M_z^\alpha, M_z^\beta$	2'2'2	[100]
	$T_{4z}^\alpha, T_{4z}^\beta$	$M_{4z}^\alpha, M_{4z}^\beta$		

TABLE XVIII. IRREPs of magnetic (M) and magnetic toroidal (MT) multipoles in the tetragonal gray point groups with twofold-rotational axes perpendicular to the primary axis or vertical reflection planes.

4/mmm1'				
IRREP	MT	M	MPG	P. axis
A _{1g} ⁻	T ₀ , T _u , T ₄ , T _{4u}		4/mmm	[001]
A _{2g} ⁻	T _{4z} ^α	M _z , M _z ^α	4/mm'm'	[001]
B _{1g} ⁻	T _v , T _{4v}	M _{xyz}	4'/mmm'	[001]
B _{2g} ⁻	T _{xy} , T _{4z} ^β	M _z ^β	4'/mm'm	[001]
E _g ⁻	T _{yz} , T _{4x} , T _{4x} ^β	M _x , M _x ^α , M _x ^β	mm'm'	[100]
	T _{zx} , T _{4y} , T _{4y} ^β	M _y , M _y ^α , M _y ^β	m'mm'	[100]
A _{1u} ⁻		M ₀ , M _u , M ₄ , M _{4u}	4/m'm'm'	[001]
A _{2u} ⁻	T _z , T _z ^α	M _{4z} ^α	4/m'mm	[001]
B _{1u} ⁻	T _{xyz}	M _v , M _{4v}	4'/m'm'm	[001]
B _{2u} ⁻	T _z ^β	M _{xy} , M _{4z} ^β	4'/m'mm'	[001]
E _u ⁻	T _x , T _x ^α , T _x ^β	M _{yz} , M _{4x} ^α , M _{4x} ^β	m'mm	[100]
	T _y , T _y ^α , T _y ^β	M _{zx} , M _{4y} ^α , M _{4y} ^β	mm'm	[100]
4221'				
IRREP	MT	M	MPG	P. axis
A ₁ ⁻	T ₀ , T _u , T ₄ , T _{4u}	M ₀ , M _u , M ₄ , M _{4u}	422	[001]
A ₂ ⁻	T _z , T _z ^α , T _{4z} ^α	M _z , M _z ^α , M _{4z} ^α	42'2'	[001]
B ₁ ⁻	T _v , T _{xyz} , T _{4v}	M _v , M _{xyz} , M _{4v}	4'22'	[001]
B ₂ ⁻	T _{xy} , T _z ^β , T _{4z} ^β	M _{xy} , M _z ^β , M _{4z} ^β	4'2'2	[001]
E ⁻	T _x , T _{yz} , T _x ^α , T _x ^β	M _x , M _{yz} , M _x ^α , M _x ^β	22'2'	[100]
	T _{4x} ^α , T _{4x} ^β	M _{4x} ^α , M _{4x} ^β		
	T _y , T _{zx} , T _y ^α , T _y ^β	M _y , M _{zx} , M _y ^α , M _y ^β	2'22'	[100]
	T _{4y} ^α , T _{4y} ^β	M _{4y} ^α , M _{4y} ^β		
4̄2m1'				
IRREP	MT	M	MPG	P. axis
A ₁ ⁻	T ₀ , T _u , T _{xyz}	M _v , M _{4v}	4̄2m	[001]
	T ₄ , T _{4u}			
A ₂ ⁻	T _z ^β , T _{4z} ^α	M _z , M _{xy} , M _z ^α , M _{4z} ^β	4̄2'm'	[001]
B ₁ ⁻	T _v , T _{4v}	M ₀ , M _u , M _{xyz}	4̄'2m'	[001]
		M ₄ , M _{4u}		
B ₂ ⁻	T _z , T _{xy} , T _z ^α , T _{4z} ^β	M _z ^β , M _{4z} ^α	4̄'2'm	[001]
E ⁻	T _x , T _{yz} , T _x ^α , T _x ^β	M _x , M _{yz} , M _x ^α , M _x ^β	22'2'	[100]
	T _{4x} ^α , T _{4x} ^β	M _{4x} ^α , M _{4x} ^β		
	T _y , T _{zx} , T _y ^α , T _y ^β	M _y , M _{zx} , M _y ^α , M _y ^β	2'22'	[100]
	T _{4y} ^α , T _{4y} ^β	M _{4y} ^α , M _{4y} ^β		
4mm1'				
IRREP	MT	M	MPG	P. axis
A ₁ ⁻	T ₀ , T _z , T _u , T _z ^α	M _{4z} ^α	4mm	[001]
	T ₄ , T _{4u}			
A ₂ ⁻	T _{4z} ^α	M ₀ , M _z , M _u , M _z ^α	4m'm'	[001]
		M ₄ , M _{4u}		
B ₁ ⁻	T _v , T _z ^β , T _{4v}	M _{xy} , M _{xyz} , M _{4z} ^β	4'mm'	[001]
B ₂ ⁻	T _{xy} , T _{xyz} , T _{4z} ^β	M _v , M _z ^β , M _{4v}	4'm'm	[001]
E ⁻	T _y , T _{yz} , T _y ^α , T _y ^β	M _x , M _{zx} , M _x ^α , M _x ^β	mm'2'	[100]
	T _{4x} ^α , T _{4x} ^β	M _{4x} ^α , M _{4x} ^β		
	T _x , T _{zx} , T _x ^α , T _x ^β	M _y , M _{yz} , M _y ^α , M _y ^β	m'm2'	[100]
	T _{4y} ^α , T _{4y} ^β	M _{4x} ^α , M _{4x} ^β		

TABLE XIX. IRREPs of magnetic (M) and magnetic toroidal (MT) multipoles in the tetragonal gray point groups without twofold-rotational axes perpendicular to the primary axis or vertical reflection planes.

4/m1'				
IRREP	MT	M	MPG	P. axis
A _g ⁻	T ₀ , T _u	M _z , M _z ^α	4/m	[001]
	T ₄ , T _{4u} , T _{4z} ^α			
B _g ⁻	T _v , T _{xy} , T _{4v} , T _{4z} ^β	M _{xyz} , M _z ^β	4'/m	[001]
E _g	T _{yz} , T _{4x} , T _{4x} ^β	M _x , M _x ^α , M _x ^β	2'/m'	[001]
	T _{zx} , T _{4y} , T _{4y} ^β	M _y , M _y ^α , M _y ^β	2'/m'	[001]
A _u ⁻	T _z , T _z ^α	M ₀ , M _u	4/m'	[001]
		M ₄ , M _{4u} , M _{4z} ^α		
B _u ⁻	T _{xyz} , T _z ^β	M _v , M _{xy} , M _{4v} , M _{4z} ^β	4'/m'	[001]
E _u	T _x , T _x ^α , T _x ^β	M _{yz} , M _{4x} ^α , M _{4x} ^β	2'/m	[001]
	T _y , T _y ^α , T _y ^β	M _{zx} , M _{4y} ^α , M _{4y} ^β	2'/m	[001]
41'				
IRREP	MT	M	MPG	P. axis
A ⁻	T ₀ , T _z , T _u , T _z ^α	M ₀ , M _z , M _u , M _z ^α	4	[001]
	T ₄ , T _{4u} , T _{4z} ^α	M ₄ , M _{4u} , M _{4z} ^α		
B ⁻	T _v , T _{xy} , T _{xyz} , T _z ^β	M _v , M _{xy} , M _{xyz} , M _z ^β	4'	[001]
	T _{4v} , T _{4z} ^β	M _{4v} , M _{4z} ^β		
E	T _x , T _{yz} , T _x ^α , T _x ^β	M _x , M _{yz} , M _x ^α , M _x ^β	2'	[001]
	T _{4x} ^α , T _{4x} ^β	M _{4x} ^α , M _{4x} ^β		
	T _y , T _{zx} , T _y ^α , T _y ^β	M _y , M _{zx} , M _y ^α , M _y ^β	2'	[001]
	T _{4y} ^α , T _{4y} ^β	M _{4y} ^α , M _{4y} ^β		
4̄1'				
IRREP	MT	M	MPG	P. axis
A ⁻	T ₀ , T _u , T _{xyz} , T _z ^β	M _z , M _v , M _{xy} , M _z ^α	4̄	[001]
	T ₄ , T _{4u} , T _{4z} ^α	M _{4v} , M _{4z} ^β		
B ⁻	T _z , T _v , T _{xy} , T _z ^α	M ₀ , M _u , M _{xyz} , M _z ^β	4̄'	[001]
	T _{4v} , T _{4z} ^β	M ₄ , M _{4u} , M _{4z} ^α		
E	T _x , T _{yz} , T _x ^α , T _x ^β	M _x , M _{yz} , M _x ^α , M _x ^β	2'	[001]
	T _{4x} ^α , T _{4x} ^β	M _{4x} ^α , M _{4x} ^β		
	T _y , T _{zx} , T _y ^α , T _y ^β	M _y , M _{zx} , M _y ^α , M _y ^β	2'	[001]
	T _{4y} ^α , T _{4y} ^β	M _{4y} ^α , M _{4y} ^β		

replace O_x^α , O_y^α , O_x^β , O_y^β with rank 3 in Eqs. (A10) and (A11) and O_{lm} with rank 4 in Eqs. (A12)–(A16) by

$$O_{3a} = \frac{\sqrt{10}}{4}x(x^2 - 3y^2), \quad (\text{A17})$$

$$O_{3b} = \frac{\sqrt{10}}{4}y(3x^2 - y^2), \quad (\text{A18})$$

$$(O_{3u}, O_{3v}) = \frac{\sqrt{6}}{4}(x(5z^2 - r^2), y(5z^2 - r^2)), \quad (\text{A19})$$

and

$$O_{40} = \frac{1}{8}(35z^4 - 30z^2r^2 + 3r^4), \quad (\text{A20})$$

$$O_{4a} = \frac{\sqrt{70}}{4}yz(3x^2 - y^2), \quad (\text{A21})$$

TABLE XX. IRREPs of magnetic (M) and magnetic toroidal (MT) multipoles in orthorhombic gray point groups.

$mmm1'$ IRREP	MT	M	MPG	P. axis
A_g^-	T_0, T_u, T_v T_4, T_{4u}, T_{4v}	M_{xyz}	mmm	[100]
B_{1g}^-	$T_{xy}, T_{4z}^\alpha, T_{4z}^\beta$	$M_z, M_z^\alpha, M_z^\beta$	$m'm'm$	[100]
B_{2g}^-	$T_{zx}, T_{4y}^\alpha, T_{4y}^\beta$	$M_y, M_y^\alpha, M_y^\beta$	$m'mm'$	[100]
B_{3g}^-	$T_{yz}, T_{4x}^\alpha, T_{4x}^\beta$	$M_x, M_x^\alpha, M_x^\beta$	$mm'm'$	[100]
A_u^-	T_{xyz}	M_0, M_u, M_v M_4, M_{4u}, M_{4v}	$m'm'm'$	[100]
B_{1u}^-	$T_z, T_z^\alpha, T_z^\beta$	$M_{xy}, M_{4z}^\alpha, M_{4z}^\beta$	mmm'	[100]
B_{2u}^-	$T_y, T_y^\alpha, T_y^\beta$	$M_{zx}, M_{4y}^\alpha, M_{4y}^\beta$	$mm'm$	[100]
B_{3u}^-	$T_x, T_x^\alpha, T_x^\beta$	$M_{yz}, M_{4x}^\alpha, M_{4x}^\beta$	$m'mm$	[100]
$2221'$ IRREP	MT	M	MPG	P. axis
A^-	T_0, T_u, T_v, T_{xyz} T_4, T_{4u}, T_{4v}	M_0, M_u, M_v, M_{xyz} M_4, M_{4u}, M_{4v}	222	[100]
B_1^-	$T_z, T_{xy}, T_z^\alpha, T_z^\beta$ $T_{4z}^\alpha, T_{4z}^\beta$	$M_z, M_{xy}, M_z^\alpha, M_z^\beta$ $M_{4z}^\alpha, M_{4z}^\beta$	2'2'2	[100]
B_2^-	$T_y, T_{zx}, T_y^\alpha, T_y^\beta$ $T_{4y}^\alpha, T_{4y}^\beta$	$M_y, M_{zx}, M_y^\alpha, M_y^\beta$ $M_{4y}^\alpha, M_{4y}^\beta$	2'22'	[100]
B_3^-	$T_x, T_{yz}, T_x^\alpha, T_x^\beta$ $T_{4x}^\alpha, T_{4x}^\beta$	$M_x, M_{yz}, M_x^\alpha, M_x^\beta$ $M_{4x}^\alpha, M_{4x}^\beta$	22'2'	[100]
$mm21'$ IRREP	MT	M	MPG	P. axis
A_1^-	T_0, T_z, T_u, T_v T_z^α, T_z^β T_4, T_{4u}, T_{4v}	M_{xy}, M_{xyz} $M_{4z}^\alpha, M_{4z}^\beta$	$mm2$	[100]
A_2^-	T_{xy}, T_{xyz} $T_{4z}^\alpha, T_{4z}^\beta$	M_0, M_z, M_u, M_v M_z^α, M_z^β M_4, M_{4u}, M_{4v}	$m'm'2$	[100]
B_1^-	$T_x, T_{zx}, T_x^\alpha, T_x^\beta$ $T_{4y}^\alpha, T_{4y}^\beta$	$M_y, M_{yz}, M_y^\alpha, M_y^\beta$ $M_{4x}^\alpha, M_{4x}^\beta$	$m'm2'$	[100]
B_2^-	$T_y, T_{yz}, T_y^\alpha, T_y^\beta$ $T_{4x}^\alpha, T_{4x}^\beta$	$M_x, M_{zx}, M_x^\alpha, M_x^\beta$ $M_{4y}^\alpha, M_{4y}^\beta$	$mm'2'$	[100]

TABLE XXI. IRREPs of magnetic (M) and magnetic toroidal (MT) multipoles in monoclinic gray point groups.

$2/m1'$ IRREP	MT	M	MPG	P. axis
A_g^-	T_0, T_u, T_v, T_{zx} T_4, T_{4u}, T_{4v} T_{4y}, T_{4y}^β	M_y $M_{xyz}, M_y^\alpha, M_y^\beta$	2/m	[010]
B_g^-	T_{yz}, T_{xy} $T_{4x}^\alpha, T_{4z}^\alpha, T_{4x}^\beta, T_{4z}^\beta$	M_x, M_z $M_x^\alpha, M_z^\alpha, M_x^\beta, M_z^\beta$	2'/m'	[010]
A_u^-	T_y $T_{xyz}, T_y^\alpha, T_y^\beta$	M_0, M_u, M_v, M_{zx} M_4, M_{4u}, M_{4v} $M_{4y}^\alpha, M_{4y}^\beta$	2/m'	[010]
B_u^-	T_x, T_z $T_x^\alpha, T_z^\alpha, T_x^\beta, T_z^\beta$	M_{yz}, M_{xy} $M_{4x}^\alpha, M_{4z}^\alpha, M_{4x}^\beta, M_{4z}^\beta$	2'/m	[010]
$21'$ IRREP	MT	M	MPG	P. axis
A^-	$T_0, T_y, T_u, T_v, T_{zx}$ $T_{xyz}, T_y^\alpha, T_y^\beta$ T_4, T_{4u}, T_{4v} T_{4y}, T_{4y}^β	$M_0, M_y, M_u, M_v, M_{zx}$ $M_{xyz}, M_y^\alpha, M_y^\beta$ M_4, M_{4u}, M_{4v} $M_{4y}^\alpha, M_{4y}^\beta$	2	[010]
B^-	T_x, T_z, T_{yz}, T_{xy} $T_x^\alpha, T_z^\alpha, T_x^\beta, T_z^\beta$ $T_{4x}^\alpha, T_{4z}^\alpha, T_{4x}^\beta, T_{4z}^\beta$	M_x, M_z, M_{yz}, M_{xy} $M_x^\alpha, M_z^\alpha, M_x^\beta, M_z^\beta$ $M_{4x}^\alpha, M_{4z}^\alpha, M_{4x}^\beta, M_{4z}^\beta$	2'	[010]
$m1'$ IRREP	MT	M	MPG	P. axis
A'^-	T_0, T_x, T_z T_u, T_v, T_{zx} $T_x^\alpha, T_z^\alpha, T_x^\beta, T_z^\beta$ T_4, T_{4u}, T_{4v} T_{4y}, T_{4y}^β	M_y, M_{yz}, M_{xy} $M_{xyz}, M_y^\alpha, M_y^\beta$ $M_{4x}^\alpha, M_{4z}^\alpha, M_{4x}^\beta, M_{4z}^\beta$	m	[010]
A''^-	T_y, T_{yz}, T_{xy} $T_{xyz}, T_y^\alpha, T_y^\beta$ $T_{4x}^\alpha, T_{4z}^\alpha, T_{4x}^\beta, T_{4z}^\beta$	M_0, M_x, M_z M_u, M_v, M_{zx} $M_x^\alpha, M_z^\alpha, M_x^\beta, M_z^\beta$ M_4, M_{4u}, M_{4v} $M_{4y}^\alpha, M_{4y}^\beta$	m'	[010]

APPENDIX B: BLACK-AND-WHITE POINT GROUP AND ITS UNITARY SUBGROUP

The type-(III) black-and-white point group $M^{(III)}$ is represented by using the type-(I) crystallographic point group G and its halving unitary subgroup H in Eq. (12); G is given by removing the prime symbol in $M^{(III)}$. The correspondence between $M^{(III)}$ and H is summarized in Table XV [26,95,145–148].

APPENDIX C: MULTIPOLE CLASSIFICATION

We present the complete tables for the multipole classification in the 32 gray point groups in Sec. C1 and 58 black-and-white point groups in Sec. C2.

1. Gray point groups

We show the M and MT multipole classification in all the 32 gray point groups in Table II in Sec. III for $m\bar{3}m1'$ and

$$O_{4b} = \frac{\sqrt{70}}{4}zx(x^2 - 3y^2), \quad (A22)$$

$$(O_{4u}^\alpha, O_{4v}^\alpha) = \frac{\sqrt{10}}{4}(zx(7z^2 - 3r^2), yz(7z^2 - 3r^2)), \quad (A23)$$

$$(O_{4u}^{\beta 1}, O_{4v}^{\beta 1}) = \frac{\sqrt{35}}{8}(x^4 - 6x^2y^2 + y^4, 4xy(x^2 - y^2)), \quad (A24)$$

$$(O_{4u}^{\beta 2}, O_{4v}^{\beta 2}) = \frac{\sqrt{5}}{4}((x^2 - y^2)(7z^2 - r^2), 2xy(7z^2 - r^2)), \quad (A25)$$

with the use of the tesseral harmonics. It is noted that three components $\{O_{xyz}, O_z^\alpha, O_z^\beta\}$ among the rank-3 functions are common to the cubic harmonics in Eqs. (A9)–(A11).

TABLE XXII. IRREPs of magnetic (M) and magnetic toroidal (MT) multipoles in triclinic gray point groups.

$\bar{1}1'$				
IRREP	MT	M	MPG	P. axis
A_g^-	T_0, T_u, T_v	M_x, M_y, M_z	$\bar{1}$	
	T_{yz}, T_{zx}, T_{xy}	$M_{xyz}, M_x^\alpha, M_y^\alpha, M_z^\alpha$		
	T_4, T_{4u}, T_{4v}	$M_x^\beta, M_y^\beta, M_z^\beta$		
	$T_{4x}^\alpha, T_{4y}^\alpha, T_{4z}^\alpha$			
	$T_{4x}^\beta, T_{4y}^\beta, T_{4z}^\beta$			
A_u^-	T_x, T_y, T_z	M_0, M_u, M_v	$\bar{1}'$	
	$T_{xyz}, T_x^\alpha, T_y^\alpha, T_z^\alpha$	M_{yz}, M_{zx}, M_{xy}		
	$T_x^\beta, T_y^\beta, T_z^\beta$	M_4, M_{4u}, M_{4v}		
		$M_{4x}^\alpha, M_{4y}^\alpha, M_{4z}^\alpha$		
		$M_{4x}^\beta, M_{4y}^\beta, M_{4z}^\beta$		
$11'$				
IRREP	MT	M	MPG	P. axis
A^-	T_0, T_x, T_y, T_z	M_0, M_x, M_y, M_z	1	
	T_u, T_v	M_u, M_v		
	T_{yz}, T_{zx}, T_{xy}	M_{yz}, M_{zx}, M_{xy}		
	$T_{xyz}, T_x^\alpha, T_y^\alpha, T_z^\alpha$	$M_{xyz}, M_x^\alpha, M_y^\alpha, M_z^\alpha$		
	$T_x^\beta, T_y^\beta, T_z^\beta$	$M_x^\beta, M_y^\beta, M_z^\beta$		
	T_4, T_{4u}, T_{4v}	M_4, M_{4u}, M_{4v}		
	$T_{4x}^\alpha, T_{4y}^\alpha, T_{4z}^\alpha$	$M_{4x}^\alpha, M_{4y}^\alpha, M_{4z}^\alpha$		
	$T_{4x}^\beta, T_{4y}^\beta, T_{4z}^\beta$	$M_{4x}^\beta, M_{4y}^\beta, M_{4z}^\beta$		

the others in Tables XVII–XXVI. The primary, secondary, and tertiary axes in Table XVI are used for the point-group operations, unless otherwise mentioned. When the primary axis is different from that in Table XVI, secondary and tertiary axes should be transformed by cyclic.

The classification for cubic systems is shown in Table XVII, tetragonal systems in Tables XVIII and XIX, orthorhombic systems in Table XX, monoclinic systems in Table XXI, triclinic systems in Table XXII, hexagonal systems in Tables XXIII and XXIV, and trigonal systems in Tables XXV and XXVI.

2. Black and white point groups

The classification of four types of multipoles, E, ET, MT, and M multipoles, in 58 black-and-white point groups is shown. The classification for cubic systems is shown in Table XXVII, tetragonal systems in Tables XXVIII and XXIX, orthorhombic systems in Table XXX, monoclinic and triclinic systems in Table XXXI, hexagonal systems in Tables XXXII and XXXIII, and trigonal systems in Table XXXIV.

APPENDIX D: COREPRESENTATION OF MAGNETIC POINT GROUPS

We give the short review of the irreducible corepresentation in magnetic point groups. For the group with $G + \mathcal{A}G$ (\mathcal{A} is the antiunitary operation), the corepresentation for the basis

TABLE XXIII. IRREPs of magnetic (M) and magnetic toroidal (MT) multipoles in the hexagonal gray point groups with twofold-rotational axes perpendicular to the primary axis or vertical reflection planes.

$6/mmm1'$				
IRREP	MT	M	MPG	P. axis
A_{1g}^-	T_0, T_u, T_{40}		$6/mmm$	[001]
A_{2g}^-		M_z, M_z^α	$6/m'm'm'$	[001]
B_{1g}^-	T_{4a}	M_{3a}	$6'/m'm'm'$	[001]
B_{2g}^-	T_{4b}	M_{3b}	$6'/m'm'm$	[001]
E_{1g}^-	T_{yz}, T_{4v}^α	M_x, M_{3u}	$mm'm'$	[100]
	T_{zx}, T_{4u}^α	M_y, M_{3v}	$m'm'm'$	[100]
E_{2g}^-	$T_v, T_{4u}^{\beta 1}, T_{4u}^{\beta 2}$	M_{xyz}	mmm	[100]
	$T_{xy}, T_{4v}^{\beta 1}, T_{4v}^{\beta 2}$	M_z^β	$m'm'm$	[100]
A_{1u}^-		M_0, M_u, M_{40}	$6/m'm'm'$	[001]
A_{2u}^-	T_z, T_z^α		$6/m'mm$	[001]
B_{1u}^-	T_{3a}	M_{4a}	$6'/mm'm$	[001]
B_{2u}^-	T_{3b}	M_{4b}	$6'/mmm'$	[001]
E_{1u}^-	T_x, T_{3u}	M_{yz}, M_{4v}^α	$m'mm$	[100]
	T_y, T_{3v}	M_{zx}, M_{4u}^α	$mm'm$	[100]
E_{2u}^-	T_{xyz}	$M_v, M_{4u}^{\beta 1}, M_{4u}^{\beta 2}$	$m'm'm'$	[100]
	T_z^β	$M_{xy}, M_{4v}^{\beta 1}, M_{4v}^{\beta 2}$	mmm'	[100]
$6221'$				
IRREP	MT	M	MPG	P. axis
A_1^-	T_0, T_u, T_{40}	M_0, M_u, M_{40}	622	[001]
A_2^-	T_z, T_z^α	M_z, M_z^α	$62'2'$	[001]
B_1^-	T_{3a}, T_{4a}	M_{3a}, M_{4a}	$6'22'$	[001]
B_2^-	T_{3b}, T_{4b}	M_{3b}, M_{4b}	$6'2'2$	[001]
E_1^-	$T_x, T_{yz}, T_{3u}, T_{4v}^\alpha$	$M_x, M_{yz}, M_{3u}, M_{4v}^\alpha$	$22'2'$	[100]
	$T_y, T_{zx}, T_{3v}, T_{4u}^\alpha$	$M_y, M_{zx}, M_{3v}, M_{4u}^\alpha$	$2'22'$	[100]
E_2^-	$T_v, T_{xyz}, T_{4u}^{\beta 1}, T_{4u}^{\beta 2}$	$M_v, M_{xyz}, M_{4u}^{\beta 1}, M_{4u}^{\beta 2}$	222	[100]
	$T_{xy}, T_z^\beta, T_{4v}^{\beta 1}, T_{4v}^{\beta 2}$	$M_{xy}, M_z^\beta, M_{4v}^{\beta 1}, M_{4v}^{\beta 2}$	$2'2'2$	[100]
$\bar{6}m21'$				
IRREP	MT	M	MPG	P. axis
$A_1'^-$	T_0, T_u, T_{3b}, T_{40}	M_{4b}	$\bar{6}m2$	[001]
$A_2'^-$	T_{3a}	M_z, M_z^α, M_{4a}	$\bar{6}m'2'$	[001]
$A_1''^-$	T_z, T_z^α, T_{4a}	M_{3a}	$\bar{6}'m2'$	[001]
$A_2''^-$	T_{4b}	M_0, M_u, M_{3b}, M_{40}	$\bar{6}'m'2$	[001]
E'^-	T_y, T_v, T_{3v}	$M_{zx}, M_{xyz}, M_{4u}^\alpha$	$m2m$	[100]
	$T_{4u}^{\beta 1}, T_{4u}^{\beta 2}$			
E''^-	T_x, T_{xy}, T_{3u}	$M_{yz}, M_z^\beta, M_{4v}^\alpha$	$m'2'm$	[100]
	$T_{4v}^{\beta 1}, T_{4v}^{\beta 2}$			
E'''^-	$T_{yz}, T_{xyz}, T_{4v}^\alpha$	M_x, M_v, M_{3u}	$m2'm'$	[100]
		$M_{4u}^{\beta 1}, M_{4u}^{\beta 2}$		
	$T_{zx}, T_z^\beta, T_{4u}^\alpha$	M_y, M_{xy}, M_{3v}	$m'2m'$	[100]
		$M_{4v}^{\beta 1}, M_{4v}^{\beta 2}$		
$6mm1'$				
IRREP	MT	M	MPG	P. axis
A_1^-	$T_0, T_z, T_u, T_z^\alpha, T_{40}$		$6mm$	[001]
A_2^-		$M_0, M_z, M_u, M_z^\alpha, M_{40}$	$6m'm'$	[001]
B_1^-	T_{3b}, T_{4a}	M_{3a}, M_{4b}	$6'mm'$	[001]
B_2^-	T_{3a}, T_{4b}	M_{3b}, M_{4a}	$6'm'm$	[001]
E_1^-	$T_y, T_{yz}, T_{3v}, T_{4v}^\alpha$	$M_x, M_{zx}, M_{3u}, M_{4u}^\alpha$	$mm'2'$	[001]
	$T_x, T_{zx}, T_{3u}, T_{4u}^\alpha$	$M_y, M_{yz}, M_{3v}, M_{4v}^\alpha$	$m'm2'$	[001]
E_2^-	$T_v, T_z^\beta, T_{4u}^{\beta 1}, T_{4u}^{\beta 2}$	$M_{xy}, M_{xyz}, M_{4u}^{\beta 1}, M_{4u}^{\beta 2}$	$mm2$	[100]
	$T_{xy}, T_{xyz}, T_{4v}^{\beta 1}, T_{4v}^{\beta 2}$	$M_v, M_z^\beta, M_{4u}^{\beta 1}, M_{4u}^{\beta 2}$	$m'm'2$	[100]

TABLE XXIV. IRREPs of magnetic (M) and magnetic toroidal (MT) multipoles in the hexagonal gray point groups without twofold-rotational axes perpendicular to the primary axis or vertical reflection planes.

$6/m1'$	IRREP	MT	M	MPG	P. axis
A_g^-		T_0, T_u, T_{40}	M_z, M_z^α	$6/m$	[001]
B_g^-		T_{4a}, T_{4b}	M_{3a}, M_{3b}	$6'/m'$	[001]
E_{1g}		T_{yz}, T_{4v}^α	M_x, M_{3u}	$2'/m'$	[001]
		T_{zx}, T_{4u}^α	M_y, M_{3v}	$2'/m'$	[001]
E_{2g}		$T_v, T_{4u}^{\beta 1}, T_{4u}^{\beta 2}$	M_{xyz}	$2/m$	[001]
		$T_{xy}, T_{4v}^{\beta 1}, T_{4v}^{\beta 2}$	M_z^β	$2/m$	[001]
A_u^-		T_z, T_z^α	M_0, M_u, M_{40}	$6/m'$	[001]
B_u^-		T_{3a}, T_{3b}	M_{4a}, M_{4b}	$6'/m$	[001]
E_{1u}		T_x, T_{3u}	M_{yz}, M_{4v}^α	$2'/m$	[001]
		T_y, T_{3v}	M_{zx}, M_{4u}^α	$2'/m$	[001]
E_{2u}		T_{xyz}	$M_v, M_{4u}^{\beta 1}, M_{4u}^{\beta 2}$	$2/m'$	[001]
		T_z^β	$M_{xy}, M_{4v}^{\beta 1}, M_{4v}^{\beta 2}$	$2/m'$	[001]
$61'$	IRREP	MT	M	MPG	P. axis
A^-		$T_0, T_z, T_u, T_z^\alpha, T_{40}$	$M_0, M_z, M_u, M_z^\alpha, M_{40}$	6	[001]
B^-		$T_{3a}, T_{3b}, T_{4a}, T_{4b}$	$M_{3a}, M_{3b}, M_{4a}, M_{4b}$	6'	[001]
E_1		$T_x, T_{yz}, T_{3u}, T_{4v}^\alpha$	$M_x, M_{yz}, M_{3u}, M_{4v}^\alpha$	2'	[001]
		$T_y, T_{zx}, T_{3v}, T_{4u}^\alpha$	$M_y, M_{zx}, M_{3v}, M_{4u}^\alpha$	2'	[001]
E_2		$T_v, T_{xyz}, T_{4u}^{\beta 1}, T_{4u}^{\beta 2}$	$M_v, M_{xyz}, M_{4u}^{\beta 1}, M_{4u}^{\beta 2}$	2	[001]
		$T_{xy}, T_z^\beta, T_{4v}^{\beta 1}, T_{4v}^{\beta 2}$	$M_{xy}, M_z^\beta, M_{4v}^{\beta 1}, M_{4v}^{\beta 2}$	2	[001]
$\bar{6}1'$	IRREP	MT	M	MPG	P. axis
A'^-		T_0, T_u	$M_z, M_z^\alpha, M_{4a}, M_{4b}$	$\bar{6}$	[001]
		T_{3a}, T_{3b}, T_{40}			
A''^-		$T_z, T_z^\alpha, T_{4a}, T_{4b}$	M_0, M_u	$\bar{6}'$	[001]
			M_{3a}, M_{3b}, M_{40}		
E'		T_x, T_v, T_{3u}	$M_{yz}, M_{xyz}, M_{4v}^\alpha$	m	[001]
		$T_{4u}^{\beta 1}, T_{4u}^{\beta 2}$			
		T_y, T_{xy}, T_{3v}	$M_{zx}, M_z^\beta, M_{4u}^\alpha$	m	[001]
		$T_{4v}^{\beta 1}, T_{4v}^{\beta 2}$			
E''		$T_{yz}, T_{xyz}, T_{4v}^\alpha$	M_x, M_v, M_{3u}	m'	[001]
			$M_{4u}^{\beta 1}, M_{4u}^{\beta 2}$		
		$T_{zx}, T_z^\beta, T_{4u}^\alpha$	M_y, M_{xy}, M_{3v}	m'	[001]
			$M_{4v}^{\beta 1}, M_{4v}^{\beta 2}$		

set of the irreducible representation Γ of \mathbf{G} , $\langle \psi |$, and another set obtained as $\langle \phi | = \mathcal{A} \langle \psi |$ is given as follows [149–151]:

$$\mathcal{R} \langle \psi, \phi | = \langle \psi, \phi | \begin{pmatrix} \Delta^\Gamma(\mathcal{R}) & 0 \\ 0 & [\Delta^\Gamma(\mathcal{A}^{-1}\mathcal{R}\mathcal{A})]^* \end{pmatrix} \text{ for } \mathcal{R} \in \mathbf{G}, \quad (\text{D1})$$

$$\mathcal{B} \langle \psi, \phi | = \langle \psi, \phi | \begin{pmatrix} 0 & \Delta^\Gamma(\mathcal{B}\mathcal{A}) \\ [\Delta^\Gamma(\mathcal{A}^{-1}\mathcal{B})]^* & 0 \end{pmatrix} \text{ for } \mathcal{B} \in \mathcal{AG}, \quad (\text{D2})$$

TABLE XXV. IRREPs of magnetic (M) and magnetic toroidal (MT) multipoles in the trigonal gray point groups with twofold-rotational axes perpendicular to the primary axis or vertical reflection planes.

$\bar{3}m1'$	IRREP	MT	M	MPG	P. axis
A_{1g}^-		T_0, T_u, T_{40}, T_{4b}	M_{3b}	$\bar{3}m$	[001]
A_{2g}^-		T_{4a}	M_z, M_z^α, M_{3a}	$\bar{3}m'$	[001]
E_g^-		T_{yz}, T_{xy}	M_x, M_{3u}, M_z^β	$2'/m'$	[010]
		$T_{4v}^\alpha, T_{4v}^{\beta 1}, T_{4v}^{\beta 2}$			
		T_{zx}, T_v	M_y, M_{3v}, M_{xyz}	$2/m$	[010]
		$T_{4u}^\alpha, T_{4u}^{\beta 1}, T_{4u}^{\beta 2}$			
A_{1u}^-		T_{3b}	M_0, M_u, M_{40}, M_{4b}	$\bar{3}'m'$	[001]
A_{2u}^-		T_z, T_z^α, T_{3a}	M_{4a}	$\bar{3}'m$	[001]
E_u^-		T_x, T_{3u}, T_z^β	M_{yz}, M_{xy}	$2'/m$	[010]
			$M_{4v}^\alpha, M_{4v}^{\beta 1}, M_{4v}^{\beta 2}$		
		T_y, T_{3v}, T_{xyz}	M_{zx}, M_v	$2/m'$	[010]
			$M_{4u}^\alpha, M_{4u}^{\beta 1}, M_{4u}^{\beta 2}$		
$321'$	IRREP	MT	M	MPG	P. axis
A_1^-		T_0, T_u, T_{3b}	M_0, M_u, M_{3b}	32	[001]
		T_{40}, T_{4b}	M_{40}, M_{4b}		
A_2^-		$T_z, T_z^\alpha, T_{3a}, T_{4a}$	$M_z, M_z^\alpha, M_{3a}, M_{4a}$	32'	[001]
E^-		T_x, T_{yz}, T_{xy}	M_x, M_{yz}, M_{xy}	2'	[010]
		T_{3u}, T_z^β	M_{3u}, M_z^β		
		$T_{4v}^\alpha, T_{4v}^{\beta 1}, T_{4v}^{\beta 2}$	$M_{4v}^\alpha, M_{4v}^{\beta 1}, M_{4v}^{\beta 2}$		
		T_y, T_{zx}, T_v	M_y, M_{zx}, M_v	2	[010]
		T_{3v}, T_{xyz}	M_{3v}, M_{xyz}		
		$T_{4u}^\alpha, T_{4u}^{\beta 1}, T_{4u}^{\beta 2}$	$M_{4u}^\alpha, M_{4u}^{\beta 1}, M_{4u}^{\beta 2}$		
$3m1'$	IRREP	MT	M	MPG	P. axis
A_1^-		$T_0, T_u, T_z, T_z^\alpha, T_{3a}$	M_{3b}, M_{4a}	3m	[001]
		T_{40}, T_{4b}			
A_2^-		T_{3b}, T_{4a}	$M_0, M_z, M_u, M_z^\alpha, M_{3a}$	3m'	[001]
			M_{40}, M_{4b}		
E^-		T_y, T_{yz}, T_{xy}	M_x, M_{zx}, M_v	m'	[010]
		T_{3v}, T_{xyz}	M_{3u}, M_z^β		
		$T_{4v}^\alpha, T_{4v}^{\beta 1}, T_{4v}^{\beta 2}$	$M_{4v}^\alpha, M_{4v}^{\beta 1}, M_{4v}^{\beta 2}$		
		T_x, T_{zx}, T_v	M_y, M_{yz}, M_{xy}	m	[010]
		T_{3u}, T_z^β	M_{3v}, M_{xyz}		
		$T_{4u}^\alpha, T_{4u}^{\beta 1}, T_{4u}^{\beta 2}$	$M_{4v}^\alpha, M_{4v}^{\beta 1}, M_{4v}^{\beta 2}$		

where \mathcal{R} (\mathcal{B}) represents the (anti)unitary point group operation and Δ^Γ is the matrix representation of Γ . In the present study, we adopt $\mathcal{A} = \theta$ for the gray point group and $\mathcal{A} = \theta\mathcal{S}$ [\mathcal{S} is the unitary point-group operation in $(\mathbf{G} - \mathbf{H})$ in Eq. (12)] for the black-and-white point group.

By the unitary transformation, we can obtain the irreducible corepresentation D^Γ [95,147,148,152–154]. The irreducible corepresentation can be classified into three

TABLE XXVI. IRREPs of magnetic (M) and magnetic toroidal (MT) multipoles in the trigonal gray point groups without twofold-rotational axes perpendicular to the primary axis or vertical reflection planes.

$\bar{3}1'$	IRREP	MT	M	MPG	P. axis
A_g^-		T_0, T_u	$M_z, M_z^\alpha, M_{3a}, M_{3b}$	$\bar{3}$	[001]
		T_{40}, T_{4a}, T_{4b}			
E_g		T_{yz}, T_{xy}	M_x, M_{3u}, M_z^β	$\bar{1}$	
		$T_{4v}^\alpha, T_{4v}^{\beta 1}, T_{4v}^{\beta 2}$			
		T_{zx}, T_v	M_y, M_{3v}, M_{xyz}	$\bar{1}$	
		$T_{4u}^\alpha, T_{4u}^{\beta 1}, T_{4u}^{\beta 2}$			
A_{1u}^-		$T_z, T_z^\alpha, T_{3a}, T_{3b}$	M_0, M_u	$\bar{3}'$	[001]
			M_{40}, M_{4a}, M_{4b}		
E_u		T_x, T_{3u}, T_z^β	M_{yz}, M_{xy}	$\bar{1}'$	
			$M_{4v}^\alpha, M_{4v}^{\beta 1}, M_{4v}^{\beta 2}$		
		T_y, T_{3v}, T_{xyz}	M_{zx}, M_v	$\bar{1}'$	
			$M_{4u}^\alpha, M_{4u}^{\beta 1}, M_{4u}^{\beta 2}$		
$31'$	IRREP	MT	M	MPG	P. axis
A^-		T_0, T_z, T_u	M_0, M_z, M_u	3	[001]
		$T_z^\alpha, T_{3a}, T_{3b}$	$M_z^\alpha, M_{3a}, M_{3b}$		
		T_{40}, T_{4a}, T_{4b}	M_{40}, M_{4a}, M_{4b}		
E		T_x, T_{yz}, T_{xy}	M_x, M_{yz}, M_{xy}	1	
		T_{3u}, T_z^β	M_{3u}, M_z^β		
		$T_{4v}^\alpha, T_{4v}^{\beta 1}, T_{4v}^{\beta 2}$	$M_{4v}^\alpha, M_{4v}^{\beta 1}, M_{4v}^{\beta 2}$		
		T_y, T_{zx}, T_v	M_y, M_{zx}, M_v	1	
		T_{3v}, T_{xyz}	M_{3v}, M_{xyz}		
		$T_{4u}^\alpha, T_{4u}^{\beta 1}, T_{4u}^{\beta 2}$	$M_{4u}^\alpha, M_{4u}^{\beta 1}, M_{4u}^{\beta 2}$		

types:

$$\sum_{\mathcal{B} \in \mathcal{AG}} \chi^\Gamma(\mathcal{B}^2) = \begin{cases} +|\mathbf{G}| & : \text{case (a),} \\ -|\mathbf{G}| & : \text{case (b),} \\ 0 & : \text{case (c),} \end{cases} \quad (\text{D3})$$

where $|\mathbf{G}|$ is the order of \mathbf{G} , and $\chi^\Gamma(\mathcal{B}^2)$ is the character with respect to the unitary operation \mathcal{B}^2 in Γ . For case (a), D^Γ is expressed as

$$D^\Gamma(\mathcal{R}) = \begin{pmatrix} \Delta^\Gamma(\mathcal{R}) & 0 \\ 0 & \Delta^\Gamma(\mathcal{R}) \end{pmatrix} \text{ for } \mathcal{R} \in \mathbf{G}, \quad (\text{D4})$$

$$D^\Gamma(\mathcal{B}) = \begin{pmatrix} \Delta^\Gamma(\mathcal{B}\mathcal{A}^{-1})N & 0 \\ 0 & -\Delta^\Gamma(\mathcal{B}\mathcal{A}^{-1})N \end{pmatrix} \text{ for } \mathcal{B} \in \mathcal{AG}, \quad (\text{D5})$$

where N is the unitary matrix to satisfy the relation $\Delta^\Gamma(\mathcal{R}) = N[\Delta^\Gamma(\mathcal{A}^{-1}\mathcal{R}\mathcal{A})]^*N^{-1}$ [95]. Here, the basis set (ψ, ϕ) is transformed by the unitary transformation

$$V = \frac{1}{\sqrt{2}} \begin{pmatrix} 1 & -1 \\ N^{-1} & N^{-1} \end{pmatrix}. \quad (\text{D6})$$

In the present paper, we denote the counterpart of the irreducible corepresentation characterized by $\Delta^\Gamma(\mathcal{R})$ for \mathcal{R} and $\pm\Delta^\Gamma(\mathcal{B}\mathcal{A}^{-1})N$ for \mathcal{B} as Γ^\pm , e.g., A_{1g}^\pm .

In contrast to case (a), the corepresentation cannot be reduced into even- and odd-parity parts with respect to the antiunitary operation in cases (b) and (c). For case (b), D^Γ is described as

$$D^\Gamma(\mathcal{R}) = \begin{pmatrix} \Delta^\Gamma(\mathcal{R}) & 0 \\ 0 & \Delta^\Gamma(\mathcal{R}) \end{pmatrix} \text{ for } \mathcal{R} \in \mathbf{G}, \quad (\text{D7})$$

$$D^\Gamma(\mathcal{B}) = \begin{pmatrix} 0 & -\Delta^\Gamma(\mathcal{B}\mathcal{A}^{-1})N \\ \Delta^\Gamma(\mathcal{B}\mathcal{A}^{-1})N & 0 \end{pmatrix} \text{ for } \mathcal{B} \in \mathcal{AG}, \quad (\text{D8})$$

where the basis set is transformed by the unitary transformation

$$U = \begin{pmatrix} 1 & 0 \\ 0 & N^{-1} \end{pmatrix}. \quad (\text{D9})$$

Meanwhile, for case (c), D^Γ is represented as

$$D^\Gamma(\mathcal{R}) = \begin{pmatrix} \Delta^\Gamma(\mathcal{R}) & 0 \\ 0 & [\Delta^\Gamma(\mathcal{A}^{-1}\mathcal{R}\mathcal{A})]^* \end{pmatrix} \text{ for } \mathcal{R} \in \mathbf{G}, \quad (\text{D10})$$

$$D^\Gamma(\mathcal{B}) = \begin{pmatrix} 0 & \Delta^\Gamma(\mathcal{B}\mathcal{A}) \\ [\Delta^\Gamma(\mathcal{A}^{-1}\mathcal{B})]^* & 0 \end{pmatrix} \text{ for } \mathcal{B} \in \mathcal{AG}. \quad (\text{D11})$$

D^Γ in both cases is not block diagonal with respect to the antiunitary operation \mathcal{B} . Thus we denote the corepresentation in cases (b) and (c) simply as Γ .

APPENDIX E: LAUE GROUP AND MAGNETIC LAUE GROUP

The correspondence between Laue groups and magnetic point groups is summarized in Table XXXV, while that between magnetic Laue groups and magnetic point groups is listed in Tables XXXVI and XXXVII. Table XXXVI presents the magnetic Laue group with the \mathcal{T} and/or \mathcal{PT} symmetry, whereas Table XXXVII presents that without the \mathcal{PT} symmetry.

APPENDIX F: DERIVATION OF MULTIPOLES IN RESPONSE TENSORS

We present the expressions of the multipoles in the response tensor components in Sec. VA. The multipoles in the rank-2 tensors are shown in Secs. F1 and F2, the rank-3 tensors in Secs. F3 and F4, and the rank-4 tensors in Secs. F5 and F6.

TABLE XXVII. IRREPs of multipoles in the cubic black-and-white point groups. Corresponding unitary subgroups are also shown. The sign \pm represents the parity with respect to the antiunitary operation in the third row, where the direction of the rotational axis or mirror plane are shown in the next row (see Appendix D). $\{X_u + iX_v, X_u - iX_v\}$ and $\{X_{4u} + iX_{4v}, X_{4u} - iX_{4v}\}$ are the basis of E representations in $m\bar{3}m'$, where $X = Q, G, T$, and M for $E_g^{(1,2)+}$, $E_u^{(1,2)+}$, $E_g^{(1,2)-}$, and $E_u^{(1,2)-}$, respectively. They are also the basis of $E^{(1,2)+}(X = Q, G)$ and $E^{(1,2)-}(X = T, M)$ in $4'32'$, whereas $E^{(1,2)+}(X = Q, M)$ and $E^{(1,2)-}(X = G, T)$ in $4'3m'$.

Magnetic point group		$m\bar{3}m$	$m\bar{3}m'$	$m\bar{3}'m'$	$4'32'$	$\bar{4}'3m'$	$m\bar{3}'$
Unitary subgroup		$\bar{4}3m$	$m\bar{3}$	432	23	23	23
Antiunitary operation		θI	$\theta C_2'$ [110]	θI	$\theta C_2'$ [110]	$\theta\sigma_d$ \perp [110]	θI
E	ET						
Q_0, Q_4		A_1^+	A_g^+	A_1^+	A^+	A^+	A^+
	G_{xyz}	A_2^+	A_g^-	A_2^+	A^-	A^-	A^+
Q_u, Q_{4u}		E^+	$E_g^{(1,2)+}$	E^+	$E^{(1,2)+}$	$E^{(1,2)+}$	E
Q_v, Q_{4v}							
Q_{4x}^α	G_x, G_x^α	T_1^+	T_g^+	T_1^+	T^+	T^+	T^+
Q_{4y}^α	G_y, G_y^α						
Q_{4z}^α	G_z, G_z^α						
Q_{yz}, Q_{4x}^β	G_x^β	T_2^+	T_g^-	T_2^+	T^-	T^-	T^+
Q_{zx}, Q_{4y}^β	G_y^β						
Q_{xy}, Q_{4z}^β	G_z^β						
	G_0, G_4	A_2^-	A_u^+	A_1^-	A^+	A^-	A^-
Q_{xyz}		A_1^-	A_u^-	A_2^-	A^-	A^+	A^-
	G_u, G_{4u}	E^-	$E_u^{(1,2)+}$	E^-	$E^{(1,2)+}$	$E^{(1,2)-}$	E
	G_v, G_{4v}						
Q_x, Q_x^α	G_{4x}	T_2^-	T_u^+	T_1^-	T^+	T^-	T^-
Q_y, Q_y^α	G_{4y}						
Q_z, Q_z^α	G_{4z}						
Q_x^β	G_{yz}, G_{4x}^β	T_1^-	T_u^-	T_2^-	T^-	T^+	T^-
Q_y^β	G_{zx}, G_{4y}^β						
Q_z^β	G_{xy}, G_{4z}^β						
MT	M						
T_0, T_4		A_1^-	A_g^-	A_1^-	A^-	A^-	A^-
	M_{xyz}	A_2^-	A_g^+	A_2^-	A^+	A^+	A^-
T_u, T_{4u}		E^-	$E_g^{(1,2)-}$	E^-	$E^{(1,2)-}$	$E^{(1,2)-}$	E
T_v, T_{4v}							
T_{4x}^α	M_x, M_x^α	T_1^-	T_g^-	T_1^-	T^-	T^-	T^-
T_{4y}^α	M_y, M_y^α						
T_{4z}^α	M_z, M_z^α						
T_{yz}, T_{4x}^β	M_x^β	T_2^-	T_g^+	T_2^-	T^+	T^+	T^-
T_{zx}, T_{4y}^β	M_y^β						
T_{xy}, T_{4z}^β	M_z^β						
	M_0, M_4	A_2^+	A_u^-	A_1^+	A^-	A^+	A^+
T_{xyz}		A_1^+	A_u^+	A_2^+	A^+	A^-	A^+
	M_u, M_{4u}	E^+	$E_u^{(1,2)-}$	E^+	$E^{(1,2)-}$	$E^{(1,2)+}$	E
	M_v, M_{4v}						
T_x, T_x^α	M_{4x}^α	T_2^+	T_u^-	T_1^+	T^-	T^+	T^+
T_y, T_y^α	M_{4y}^α						
T_z, T_z^α	M_{4z}^α						
T_x^β	M_{yz}, M_{4x}^β	T_1^+	T_u^+	T_2^+	T^+	T^-	T^+
T_y^β	M_{zx}, M_{4y}^β						
T_z^β	M_{xy}, M_{4z}^β						

TABLE XXVIII. IRREPs of multipoles in tetragonal black-and-white point groups except for $4'/m'$, $4/m'$, $4'/m$, $\bar{4}'$, and $4'$ (see also Table XXIX). $\{X_x + iX_y, X_x - iX_y\}$, $\{X_{yz} - iX_{zx}, X_{yz} + iX_{zx}\}$, $\{X_x^\alpha + iX_y^\alpha, X_x^\alpha - iX_y^\alpha\}$, $\{X_x^\beta - iX_y^\beta, X_x^\beta + iX_y^\beta\}$, $\{X_{4x}^\alpha + iX_{4y}^\alpha, X_{4x}^\alpha - iX_{4y}^\alpha\}$, and $\{X_{4x}^\beta - iX_{4y}^\beta, X_{4x}^\beta + iX_{4y}^\beta\}$ ($X = Q, G, T, M$) are the basis of $E_{g/u}^{(1,2)\pm}$ in $4/m'm'm'$, and $E^{(1,2)\pm}$ in $42'2'$, $4m'm'$, and $\bar{4}2'm'$.

Magnetic point group		$4/m'm'm'$	$4/m'mm$	$4'/m'm'm'$	$4/mm'm'$	$4'/mm'm'$	$42'2'$	$4'22'$	$4m'm'$	$4'mm'$	$\bar{4}2'm'$	$\bar{4}'m2'$	$\bar{4}'2m'$
Unitary subgroup		422	4mm	$\bar{4}2m$	4/m	mmm	4	222	4	mm2	$\bar{4}$	mm2	222
Antiuunitary operation		θI	θI	θI	$\theta C_2'$ [100]	$\theta C_2''$ [110]	$\theta C_2'$ [100]	$\theta C_2''$ [110]	$\theta\sigma_v$ \perp [100]	$\theta\sigma_d$ \perp [110]	$\theta C_2'$ [100]	$\theta C_2''$ [110]	$\theta\sigma_d$ \perp [110]
E	ET												
$Q_0, Q_u,$ Q_4, Q_{4u}		A_1^+	A_1^+	A_1^+	A_g^+	A_g^+	A^+	A^+	A^+	A_1^+	A^+	A_1^+	A^+
Q_v, Q_{4v}	G_{xyz}	B_1^+	B_1^+	B_1^+	B_g^+	A_g^-	B^+	A^-	B^+	A_1^-	B^+	A_1^-	A^-
$Q_{yz}, Q_{4x}, Q_{4x}^\beta$	$G_x, G_x^\alpha, G_x^\beta$	E^+	E^+	E^+	$E_g^{(1,2)+}$	B_{2g}	$E^{(1,2)+}$	B_2	$E^{(1,2)+}$	B_1	$E^{(1,2)+}$	B_1	B_2
$Q_{zx}, Q_{4y}, Q_{4y}^\beta$	$G_y, G_y^\alpha, G_y^\beta$												
Q_{4z}^α	G_z, G_z^α	A_2^+	A_2^+	A_2^+	A_g^-	B_{1g}^-	A^-	B_1^-	A^-	A_2^-	A^-	A_2^-	B_1^-
Q_{xy}, Q_{4z}^β	G_z^β	B_2^+	B_2^+	B_2^+	B_g^-	B_{1g}^+	B^-	B_1^+	B^-	A_2^+	B^-	A_2^+	B_1^+
	$G_0, G_u,$ G_4, G_{4u}	A_1^-	A_2^-	B_1^-	A_u^+	A_u^+	A^+	A^+	A^-	A_2^-	B^+	A_2^+	A^-
Q_{xyz}	G_v, G_{4v}	B_1^-	B_2^-	A_1^-	B_u^+	A_u^-	B^+	A^-	B^-	A_2^+	A^+	A_2^-	A^+
$Q_x, Q_x^\alpha, Q_x^\beta$	$G_{yz}, G_{4x}^\alpha, G_{4x}^\beta$	E^-	E^-	E^-	$E_u^{(1,2)+}$	B_{2u}	$E^{(1,2)+}$	B_2	$E^{(1,2)-}$	B_1	$E^{(2,1)+}$	B_1	B_2
$Q_y, Q_y^\alpha, Q_y^\beta$	$G_{zx}, G_{4y}^\alpha, G_{4y}^\beta$												
Q_z, Q_z^α	G_{4z}^α	A_2^-	A_1^-	B_2^-	A_u^-	B_{1u}^-	A^-	B_1^-	A^+	A_1^+	B^-	A_1^-	B_1^+
Q_z^β	G_{xy}, G_{4z}^β	B_2^-	B_1^-	A_2^-	B_u^-	B_{1u}^+	B^-	B_1^+	B^+	A_1^-	A^-	A_1^+	B_1^-
MT	M												
$T_0, T_u,$ T_4, T_{4u}		A_1^-	A_1^-	A_1^-	A_g^-	A_g^-	A^-	A^-	A^-	A_1^-	A^-	A_1^-	A^-
T_v, T_{4v}	M_{xyz}	B_1^-	B_1^-	B_1^-	B_g^-	A_g^+	B^-	A^+	B^-	A_1^+	B^-	A_1^+	A^+
$T_{yz}, T_{4x}, T_{4x}^\beta$	$M_x, M_x^\alpha, M_x^\beta$	E^-	E^-	E^-	$E_g^{(1,2)-}$	B_{2g}	$E^{(1,2)-}$	B_2	$E^{(1,2)-}$	B_1	$E^{(1,2)-}$	B_1	B_2
$T_{zx}, T_{4y}, T_{4y}^\beta$	$M_y, M_y^\alpha, M_y^\beta$												
T_{4z}^α	M_z, M_z^α	A_2^-	A_2^-	A_2^-	A_g^+	B_{1g}^+	A^+	B_1^+	A^+	A_2^+	A^+	A_2^+	B_1^+
T_{xy}, T_{4z}^β	M_z^β	B_2^-	B_2^-	B_2^-	B_g^+	B_{1g}^-	B^+	B_1^-	B^+	A_2^-	B^+	A_2^-	B_1^-
	$M_0, M_u,$ M_4, M_{4u}	A_1^+	A_2^+	B_1^+	A_u^-	A_u^-	A^-	A^-	A^+	A_2^+	B^-	A_2^-	A^+
T_{xyz}	M_v, M_{4v}	B_1^+	B_2^+	A_1^+	B_u^-	A_u^+	B^-	A^+	B^+	A_2^-	A^-	A_2^+	A^-
$T_x, T_x^\alpha, T_x^\beta$	$M_{yz}, M_{4x}^\alpha, M_{4x}^\beta$	E^+	E^+	E^+	$E_u^{(1,2)-}$	B_{2u}	$E^{(1,2)-}$	B_2	$E^{(1,2)+}$	B_1	$E^{(2,1)-}$	B_1	B_2
$T_y, T_y^\alpha, T_y^\beta$	$M_{zx}, M_{4y}^\alpha, M_{4y}^\beta$												
T_z, T_z^α	M_{4z}^α	A_2^+	A_1^+	B_2^+	A_u^+	B_{1u}^+	A^+	B_1^+	A^-	A_1^-	B^+	A_1^+	B_1^-
T_z^β	M_{xy}, M_{4z}^β	B_2^+	B_1^+	A_2^+	B_u^+	B_{1u}^-	B^+	B_1^-	B^-	A_1^+	A^+	A_1^-	B_1^+

1. $\chi^{[1 \times 1]}$

We decompose the rank-2 tensor $\chi^{[1 \times 1]}$ into the monopole, dipole, and quadrupole components, which are given as

$$\chi^{M(1 \times 1)} = \frac{1}{3} \sum_i \chi_{ii}^{[1 \times 1]}, \quad (F1)$$

$$\chi_i^{D(1 \times 1)} = \frac{1}{2} \sum_{jk} \epsilon_{ijk} \chi_{jk}^{[1 \times 1]}, \quad (F2)$$

$$\chi_{ij}^{Q(1 \times 1)} = \frac{1}{2} (\chi_{i,j}^{[1 \times 1]} + \chi_{j,i}^{[1 \times 1]}) = \chi_{ji}^{Q(1 \times 1)}, \quad (F3)$$

TABLE XXIX. IRREPs of multipoles in tetragonal black-and-white point groups for $4'/m'$, $4/m'$, $4'/m$, $\bar{4}'$, and $4'$.

Magnetic point group	$4'/m'$	$4/m'$	$4'/m$	$\bar{4}'$	$4'$
Unitary subgroup	$\bar{4}$	4	$2/m$	2	2
Antiunitary operation	θI	θI	θC_4 [001]	θIC_4 [001]	θC_4 [001]
E	ET				
$Q_0, Q_u, Q_4, Q_{4u}, Q_{4z}^\alpha$	G_z, G_z^α	A ⁺	A ⁺	A _g ⁺	A ⁺
$Q_v, Q_{xy}, Q_{4v}, Q_{4z}^\beta$	G_{xyz}, G_z^β	B ⁺	B ⁺	A _g ⁻	A ⁻
$Q_{yz}, Q_{4x}^\alpha, Q_{4x}^\beta$	$G_x, G_x^\alpha, G_x^\beta$	E	E	B _g	B
$Q_{zx}, Q_{4y}^\alpha, Q_{4y}^\beta$	$G_y, G_y^\alpha, G_y^\beta$				
Q_z, Q_z^α	$G_0, G_u, G_4, G_{4u}, G_{4z}^\alpha$	B ⁻	A ⁻	A _u ⁺	A ⁻
Q_{xyz}, Q_z^β	$G_v, G_{xy}, G_{4v}, G_{4z}^\beta$	A ⁻	B ⁻	A _u ⁻	A ⁻
$Q_x, Q_x^\alpha, Q_x^\beta$	$G_{yz}, G_{4x}^\alpha, G_{4x}^\beta$	E	E	B _u	B
$Q_y, Q_y^\alpha, Q_y^\beta$	$G_{zx}, G_{4y}^\alpha, G_{4y}^\beta$				
MT	M				
$T_0, T_u, T_4, T_{4u}, T_{4z}^\alpha$	M_z, M_z^α	A ⁻	A ⁻	A _g ⁻	A ⁻
$T_v, T_{xy}, T_{4v}, T_{4z}^\beta$	M_{xyz}, M_z^β	B ⁻	B ⁻	A _g ⁺	A ⁺
$T_{yz}, T_{4x}^\alpha, T_{4x}^\beta$	$M_x, M_x^\alpha, M_x^\beta$	E	E	B _g	B
$T_{zx}, T_{4y}^\alpha, T_{4y}^\beta$	$M_y, M_y^\alpha, M_y^\beta$				
T_z, T_z^α	$M_0, M_u, M_4, M_{4u}, M_{4z}^\alpha$	B ⁺	A ⁺	A _u ⁻	A ⁺
T_{xyz}, T_z^β	$M_v, M_{xy}, M_{4v}, M_{4z}^\beta$	A ⁺	B ⁺	A _u ⁺	A ⁻
$T_x, T_x^\alpha, T_x^\beta$	$M_{yz}, M_{4x}^\alpha, M_{4x}^\beta$	E	E	B _u	B
$T_y, T_y^\alpha, T_y^\beta$	$M_{zx}, M_{4y}^\alpha, M_{4y}^\beta$				

TABLE XXX. IRREPs of multipoles in orthorhombic black-and-white point groups.

Magnetic point group	$m'm'm'$	mmm'	$m'm'm$	$2'2'2$	$m'm'2$	$m'm'2'$
Unitary subgroup	222	$mm2$	$2/m$	2	2	m
Antiunitary operation	θI	θI	θC_{2x}	θC_{2x}	$\theta \sigma_x$	θC_{2z}
E	ET					
$Q_0, Q_u, Q_v, Q_4, Q_{4u}, Q_{4v}$	G_{xyz}	A ⁺	A ₁ ⁺	A _g ⁺	A ⁺	A ⁺
$Q_{yz}, Q_{4x}^\alpha, Q_{4x}^\beta$	$G_x, G_x^\alpha, G_x^\beta$	B ₃ ⁺	B ₂ ⁺	B _g ⁺	B ⁺	A ^{''-}
$Q_{zx}, Q_{4y}^\alpha, Q_{4y}^\beta$	$G_y, G_y^\alpha, G_y^\beta$	B ₂ ⁺	B ₁ ⁺	B _g ⁻	B ⁻	A ^{'-}
$Q_{xy}, Q_{4z}^\alpha, Q_{4z}^\beta$	$G_z, G_z^\alpha, G_z^\beta$	B ₁ ⁺	A ₂ ⁺	A _g ⁻	A ⁻	A ^{''+}
Q_{xyz}	$G_0, G_u, G_v, G_4, G_{4u}, G_{4v}$	A ⁻	A ₂ ⁻	A _u ⁺	A ⁺	A ^{''+}
$Q_x, Q_x^\alpha, Q_x^\beta$	$G_{yz}, G_{4x}^\alpha, G_{4x}^\beta$	B ₃ ⁻	B ₁ ⁻	B _u ⁺	B ⁺	A ^{'-}
$Q_y, Q_y^\alpha, Q_y^\beta$	$G_{zx}, G_{4y}^\alpha, G_{4y}^\beta$	B ₂ ⁻	B ₂ ⁻	B _u ⁻	B ⁻	A ^{''-}
$Q_z, Q_z^\alpha, Q_z^\beta$	$G_{xy}, G_{4z}^\alpha, G_{4z}^\beta$	B ₁ ⁻	A ₁ ⁻	A _u ⁻	A ⁻	A ^{''+}
MT	M					
$T_0, T_u, T_v, T_4, T_{4u}, T_{4v}$	M_{xyz}	A ⁻	A ₁ ⁻	A _g ⁻	A ⁻	A ^{'-}
$T_{yz}, T_{4x}^\alpha, T_{4x}^\beta$	$M_x, M_x^\alpha, M_x^\beta$	B ₃ ⁻	B ₂ ⁻	B _g ⁻	B ⁻	A ^{''+}
$T_{zx}, T_{4y}^\alpha, T_{4y}^\beta$	$M_y, M_y^\alpha, M_y^\beta$	B ₂ ⁻	B ₁ ⁻	B _g ⁺	B ⁺	A ^{''+}
$T_{xy}, T_{4z}^\alpha, T_{4z}^\beta$	$M_z, M_z^\alpha, M_z^\beta$	B ₁ ⁻	A ₂ ⁻	A _g ⁺	A ⁺	A ^{''-}
T_{xyz}	$M_0, M_u, M_v, M_4, M_{4u}, M_{4v}$	A ⁺	A ₂ ⁺	A _u ⁻	A ⁻	A ^{''-}
$T_x, T_x^\alpha, T_x^\beta$	$M_{yz}, M_{4x}^\alpha, M_{4x}^\beta$	B ₃ ⁺	B ₁ ⁺	B _u ⁻	B ⁻	A ^{''+}
$T_y, T_y^\alpha, T_y^\beta$	$M_{zx}, M_{4y}^\alpha, M_{4y}^\beta$	B ₂ ⁺	B ₂ ⁺	B _u ⁺	B ⁺	A ^{''+}
$T_z, T_z^\alpha, T_z^\beta$	$M_{xy}, M_{4z}^\alpha, M_{4z}^\beta$	B ₁ ⁺	A ₁ ⁺	A _u ⁺	A ⁺	A ^{'-}

TABLE XXXI. IRREPs of multipoles in monoclinic and triclinic black-and-white point groups.

Magnetic point group	$2'/m$	$2/m'$	$2'/m'$	$2'$	m'	$\bar{1}'$
Unitary subgroup	m	2	$\bar{1}$	1	1	1
Antiunitary operation	θI	θI	θC_2	θC_2	$\theta\sigma$	θI
E	ET					
$Q_0, Q_u, Q_v, Q_{zx}, Q_4, Q_{4u}, Q_{4v}, Q_{4y}^\alpha, Q_{4y}^\beta$	$G_y, G_{xyz}, G_y^\alpha, G_y^\beta$	A'^+	A^+	A_g^+	A^+	A^+
$Q_{yz}, Q_{xy}, Q_{4x}^\alpha, Q_{4z}^\alpha, Q_{4x}^\beta, Q_{4z}^\beta$	$G_x, G_z, G_x^\alpha, G_z^\alpha, G_x^\beta, G_z^\beta$	A''^+	B^+	A_g^-	A^-	A^+
$Q_y, Q_{xyz}, Q_y^\alpha, Q_y^\beta$	$G_0, G_u, G_v, G_{zx}, G_4, G_{4u}, G_{4v}, G_{4y}^\alpha, G_{4y}^\beta$	A''^-	A^-	A_u^+	A^+	A^-
$Q_x, Q_z, Q_x^\alpha, Q_z^\alpha, Q_x^\beta, Q_z^\beta$	$G_{yz}, G_{xy}, G_{4x}^\alpha, G_{4z}^\alpha, G_{4x}^\beta, G_{4z}^\beta$	A'^-	B^-	A_u^-	A^-	A^+
MT	M					
$T_0, T_u, T_v, T_{zx}, T_4, T_{4u}, T_{4v}, T_{4y}^\alpha, T_{4y}^\beta$	$M_y, M_{xyz}, M_y^\alpha, M_y^\beta$	A'^-	A^-	A_g^-	A^-	A^-
$T_{yz}, T_{xy}, T_{4x}^\alpha, T_{4z}^\alpha, T_{4x}^\beta, T_{4z}^\beta$	$M_x, M_z, M_x^\alpha, M_z^\alpha, M_x^\beta, M_z^\beta$	A''^-	B^-	A_g^+	A^+	A^-
$T_y, T_{xyz}, T_y^\alpha, T_y^\beta$	$M_0, M_u, M_v, M_{zx}, M_4, M_{4u}, M_{4v}, M_{4y}^\alpha, M_{4y}^\beta$	A''^+	A^+	A_u^-	A^-	A^+
$T_x, T_z, T_x^\alpha, T_z^\alpha, T_x^\beta, T_z^\beta$	$M_{yz}, M_{xy}, M_{4x}^\alpha, M_{4z}^\alpha, M_{4x}^\beta, M_{4z}^\beta$	A'^+	B^+	A_u^+	A^+	A^+

respectively ($i, j = x, y, z$). ϵ_{ijk} is the totally antisymmetric tensor (Levi-Civita symbol). The upper script of $\chi^{X(l_B \times l_F)}$ represents the ranks of the response (output), l_B , and the external field (input), l_F , in terms of the spherical tensors. By using Eqs. (F1)–(F3), the multipoles in Eq. (20) are expressed as

$$X_0 = \chi^{M(1 \times 1)}, \quad (F4)$$

$$(Y_x, Y_y, Y_z) = (\chi_x^{D(1 \times 1)}, \chi_y^{D(1 \times 1)}, \chi_z^{D(1 \times 1)}), \quad (F5)$$

$$X_u = \frac{1}{6} \left(3\chi_{zz}^{Q(1 \times 1)} - \sum_i \chi_{ii}^{Q(1 \times 1)} \right), \quad X_v = \frac{1}{2} (\chi_{xx}^{Q(1 \times 1)} - \chi_{yy}^{Q(1 \times 1)}), \quad (X_{yz}, X_{zx}, X_{xy}) = (\chi_{yz}^{Q(1 \times 1)}, \chi_{zx}^{Q(1 \times 1)}, \chi_{xy}^{Q(1 \times 1)}). \quad (F6)$$

2. $\chi^{[0 \times 2]}$

$\chi^{[0 \times 2]}$ is decomposed into the monopole and quadrupole in Eq. (21), which are represented by

$$X_0 = \frac{1}{3} (\chi_{0:xx}^{[0 \times 2]} + \chi_{0:yy}^{[0 \times 2]} + \chi_{0:zz}^{[0 \times 2]}), \quad (F7)$$

$$X_u = \frac{1}{6} \left(3\chi_{0:zz}^{[0 \times 2]} - \sum_i \chi_{0:ii}^{[0 \times 2]} \right), \quad X_v = \frac{1}{2} (\chi_{0:xx}^{[0 \times 2]} - \chi_{0:yy}^{[0 \times 2]}), \quad (X_{yz}, X_{zx}, X_{xy}) = (\chi_{0:yz}^{[0 \times 2]}, \chi_{0:zx}^{[0 \times 2]}, \chi_{0:xy}^{[0 \times 2]}). \quad (F8)$$

3. $\chi^{[1 \times 2]}$

$\chi^{[1 \times 2]}$ consists of the dipole, quadrupole, and octupole components, which are represented by using the component $\chi_{i;jk}^{[1 \times 2]}$ ($= \chi_{i;jk}^{[1 \times 2]}$) as

$$\chi_i^{D(1 \times 0)} = \frac{1}{3} \sum_j \chi_{i;jj}^{[1 \times 2]}, \quad (F9)$$

$$\chi_i^{D(1 \times 2)} = \sum_j \left(\frac{1}{3} \chi_{i;jj}^{[1 \times 2]} - \chi_{j;ij}^{[1 \times 2]} \right), \quad (F10)$$

$$\chi_{ij}^{Q(1 \times 2)} = \frac{1}{2} \sum_{kl} (\epsilon_{ikl} \chi_{k;l j}^{[1 \times 2]} + \epsilon_{jkl} \chi_{k;l i}^{[1 \times 2]}) = \chi_{ji}^{Q(1 \times 2)}, \quad (F11)$$

$$\chi_{ijk}^{O(1 \times 2)} = \frac{1}{3} (\chi_{i;jk}^{[1 \times 2]} + \chi_{j;ki}^{[1 \times 2]} + \chi_{k;ij}^{[1 \times 2]}) = \chi_{jki}^{O(1 \times 2)} = \chi_{jik}^{O(1 \times 2)}. \quad (F12)$$

It is noted that there are two dipole components in $\chi^{[1 \times 2]}$, as the symmetric tensor field $F^{[2]} = (F_{xx}, F_{yy}, F_{zz}, F_{yz}, F_{zx}, F_{xy})$ is decomposed into the components with $l_F = 0$ and with $l_F = 2$. The $l_F = 0$ component in $F^{[2]}$ leads to $\chi_i^{D(1 \times 0)}$ in Eq. (F9), and the $l_F = 2$ component in $F^{[2]}$ leads to $\chi_i^{D(1 \times 2)}$, $\chi_{ij}^{Q(1 \times 2)}$, and $\chi_{ijk}^{O(1 \times 2)}$ in Eqs. (F10)–(F12).

TABLE XXXII. IRREPs of multipoles in hexagonal black-and-white point groups except for $6'/m$, $6/m'$, $6'/m'$, $\bar{6}'$, and $6'$ (see also Table XXXIII). $\{X_x - iX_y, X_x + iX_y\}$, $\{X_{yz} + iX_{zx}, X_{yz} - iX_{zx}\}$, $\{X_v + iX_{xy}, X_v - iX_{xy}\}$, $\{X_{3u} - iX_{3v}, X_{3u} + iX_{3v}\}$, $\{X_{xyz} - iX_z^\beta, X_{xyz} + iX_z^\beta\}$, $\{X_{4v}^\alpha + iX_{4u}^\alpha, X_{4v}^\alpha - iX_{4u}^\alpha\}$, $\{X_{4u}^{\beta 1} - iX_{4v}^{\beta 1}, X_{4u}^{\beta 1} + iX_{4v}^{\beta 1}\}$, and $\{X_{4u}^{\beta 2} + iX_{4v}^{\beta 2}, X_{4u}^{\beta 2} - iX_{4v}^{\beta 2}\}$ ($X = Q, G, M, T$) are the basis of $E_{1g/u}^{(1,2)\pm}$ and $E_{2g/u}^{(1,2)\pm}$ representations in $6/mmm'$, $E_1^{(1,2)\pm}$ and $E_2^{(1,2)\pm}$ representations in $62'2'$ and $6m'm'$, and $E^{(1,2)\pm}$ and $E''^{(1,2)\pm}$ representations in $\bar{6}m'2'$.

Magnetic point group		$6/m'm'm'$	$6/m'mm$	$6'/mmm'$	$6/mn'm'$	$6'/m'mm'$	$62'2'$	$6'22'$	$6m'm'$	$6'mm'$	$\bar{6}m'2'$	$\bar{6}'m2'$	$\bar{6}'m'2'$
Unitary subgroup		622	6mm	$\bar{6}m2$	$6/m$	$\bar{3}m$	6	32	6	3m	$\bar{6}$	3m	32
Antiuunitary operation		θI	θI	θI	θC_{2x}	θC_2	θC_{2x}	θC_2	$\theta \sigma_x$	θC_2	θC_{2y}	$\theta \sigma_h$	$\theta \sigma_h$
E	ET												
Q_0, Q_u, Q_{40}	G_z, G_z^α	A_1^+	A_1^+	A_1^{++}	A_g^+	A_{1g}^+	A^+	A_1^+	A^+	A_1^+	A^{++}	A_1^+	A_1^+
Q_{4a}	G_{3a}	A_2^+	A_2^+	A_2^{++}	A_g^-	A_{2g}^+	A^-	A_2^+	A^-	A_2^+	A^{--}	A_2^+	A_2^+
Q_{4b}	G_{3b}	B_1^+	B_1^+	A_1^{++}	B_g^+	A_{1g}^-	B^+	A_1^-	B^+	A_1^-	A^{--}	A_1^-	A_2^-
Q_{yz}, Q_{4v}^α	G_x, G_{3u}	B_2^+	B_2^+	A_1^{++}	B_g^-	A_{2g}^-	B^-	A_2^-	B^-	A_2^-	A^{++}	A_2^-	A_1^-
Q_{zx}, Q_{4u}^α	G_y, G_{3v}	E_1^+	E_1^+	E''^+	$E_{1g}^{(1,2)+}$	E_g^-	$E_1^{(1,2)+}$	E^-	$E_1^{(1,2)+}$	E^-	$E''^{(1,2)-}$	E^-	E^-
$Q_v, Q_{4u}^{\beta 1}, Q_{4u}^{\beta 2}$	G_{xyz}	E_2^+	E_2^+	E^+	$E_{2g}^{(1,2)+}$	E_g^+	$E_2^{(1,2)+}$	E^+	$E_2^{(1,2)+}$	E^+	$E^{(1,2)+}$	E^+	E^+
$Q_{xy}, Q_{4v}^{\beta 1}, Q_{4v}^{\beta 2}$	G_z^β												
	G_0, G_u, G_{40}	A_1^-	A_2^-	$A_1''^-$	A_u^+	A_{1u}^+	A^+	A_1^+	A^-	A_2^+	A^{++}	A_2^-	A_1^-
Q_z, Q_z^α		A_2^-	A_1^-	$A_2''^-$	A_u^-	A_{2u}^+	A^-	A_2^+	A^+	A_1^+	A^{--}	A_1^-	A_2^-
Q_{3a}	G_{4a}	B_1^-	B_2^-	$A_2''^-$	B_u^+	A_{1u}^-	B^+	A_1^-	B^-	A_2^-	A^{--}	A_2^+	A_2^+
Q_{3b}	G_{4b}	B_2^-	B_1^-	$A_1''^-$	B_u^-	A_{2u}^-	B^-	A_2^-	B^+	A_1^-	A^{++}	A_1^+	A_1^+
Q_x, Q_{3u}	G_{yz}, G_{4v}^α	E_1^-	E_1^-	E'^-	$E_{1u}^{(1,2)+}$	E_u^-	$E_1^{(1,2)+}$	E^-	$E_1^{(1,2)-}$	E^-	$E^{(1,2)-}$	E^+	E^+
Q_y, Q_{3v}	G_{zx}, G_{4u}^α												
Q_{xyz}	$G_v, G_{4u}^{\beta 1}, G_{4u}^{\beta 2}$	E_2^-	E_2^-	E''^-	$E_{2u}^{(1,2)+}$	E_u^+	$E_2^{(1,2)+}$	E^+	$E_2^{(1,2)-}$	E^+	$E''^{(1,2)+}$	E^-	E^-
Q_z^β	$G_{xy}, G_{4v}^{\beta 1}, G_{4v}^{\beta 2}$												
MT	M												
T_0, T_u, T_{40}		A_1^-	A_1^-	$A_1'^-$	A_g^-	A_{1g}^-	A^-	A_1^-	A^-	A_1^-	A^{--}	A_1^-	A_1^-
	M_z, M_z^α	A_2^-	A_2^-	$A_2'^-$	A_g^+	A_{2g}^-	A^+	A_2^-	A^+	A_2^-	A^{++}	A_2^-	A_2^-
T_{4a}	M_{3a}	B_1^-	B_1^-	$A_2'^-$	B_g^-	A_{1g}^+	B^-	A_1^+	B^-	A_1^+	A^{++}	A_1^+	A_2^+
T_{4b}	M_{3b}	B_2^-	B_2^-	$A_1'^-$	B_g^+	A_{2g}^+	B^+	A_2^+	B^+	A_2^+	A^{--}	A_2^+	A_1^+
T_{yz}, T_{4v}^α	M_x, M_{3u}	E_1^-	E_1^-	E''^-	$E_{1g}^{(1,2)-}$	E_g^+	$E_1^{(1,2)-}$	E^+	$E_1^{(1,2)-}$	E^+	$E''^{(1,2)+}$	E^+	E^+
T_{zx}, T_{4u}^α	M_y, M_{3v}												
$T_v, T_{4u}^{\beta 1}, T_{4u}^{\beta 2}$	M_{xyz}	E_2^-	E_2^-	E'^-	$E_{2g}^{(1,2)-}$	E_g^-	$E_2^{(1,2)-}$	E^-	$E_2^{(1,2)-}$	E^-	$E^{(1,2)-}$	E^-	E^-
$T_{xy}, T_{4v}^{\beta 1}, T_{4v}^{\beta 2}$	M_z^β												
	M_0, M_u, M_{40}	A_1^+	A_2^+	A_1^{++}	A_u^-	A_{1u}^-	A^-	A_1^-	A^+	A_2^-	A^{--}	A_2^+	A_1^+
T_z, T_z^α		A_2^+	A_1^+	A_2^{++}	A_u^+	A_{2u}^-	A^+	A_2^-	A^-	A_1^-	A^{++}	A_1^+	A_2^+
T_{3a}	M_{4a}	B_1^+	B_2^+	A_2^+	B_u^-	A_{1u}^+	B^-	A_1^+	B^+	A_2^+	A^{++}	A_2^-	A_2^-
T_{3b}	M_{4b}	B_2^+	B_1^+	A_1^+	B_u^+	A_{2u}^+	B^+	A_2^+	B^-	A_1^+	A^{--}	A_1^-	A_1^-
T_x, T_{3u}	M_{yz}, M_{4v}^α	E_1^+	E_1^+	E^+	$E_{1u}^{(1,2)-}$	E_u^+	$E_1^{(1,2)-}$	E^+	$E_1^{(1,2)+}$	E^+	$E^{(1,2)+}$	E^-	E^-
T_y, T_{3v}	M_{zx}, M_{4u}^α												
T_{xyz}	$M_v, M_{4u}^{\beta 1}, M_{4u}^{\beta 2}$	E_2^+	E_2^+	E''^+	$E_{2u}^{(1,2)-}$	E_u^-	$E_2^{(1,2)-}$	E^-	$E_2^{(1,2)+}$	E^-	$E''^{(1,2)-}$	E^+	E^+
T_z^β	$M_{xy}, M_{4v}^{\beta 1}, M_{4v}^{\beta 2}$												

The corresponding multipoles in Eq. (22) are expressed by $\chi_i^{D(1 \times 0)}$, $\chi_i^{D(1 \times 2)}$, $\chi_{ij}^{Q(1 \times 2)}$, and $\chi_{ijk}^{O(1 \times 2)}$ in Eqs. (F9)–(F12) as

$$(Y_x, Y_y, Y_z) = \frac{1}{10}(\chi_x^{D(1 \times 2)}, \chi_y^{D(1 \times 2)}, \chi_z^{D(1 \times 2)}), \quad (F13)$$

$$(Y'_x, Y'_y, Y'_z) = (\chi_x^{D(1 \times 0)}, \chi_y^{D(1 \times 0)}, \chi_z^{D(1 \times 0)}), \quad (F14)$$

$$X_u = \frac{1}{6} \left(3\chi_{zz}^{Q(1 \times 2)} - \sum_i \chi_{ii}^{Q(1 \times 2)} \right), \quad X_v = \frac{1}{6} (\chi_{xx}^{Q(1 \times 2)} - \chi_{yy}^{Q(1 \times 2)}), \quad (X_{yz}, X_{zx}, X_{xy}) = \frac{1}{3} (\chi_{yz}^{Q(1 \times 2)}, \chi_{zx}^{Q(1 \times 2)}, \chi_{xy}^{Q(1 \times 2)}), \quad (F15)$$

TABLE XXXIII. IRREPs of multipoles in hexagonal black-and-white point groups for $6'/m$, $6/m'$, $6'/m'$, $\bar{6}'$, and $6'$.

Magnetic point group		$6'/m$	$6/m'$	$6'/m'$	$\bar{6}'$	$6'$
Unitary subgroup		$\bar{6}$	6	$\bar{3}$	3	3
Antiunitary operation		θI	θI	θC_2	$\theta \sigma_h$	θC_2
E	ET					
Q_0, Q_u, Q_{40}	G_z, G_z^α	$A^{'+}$	A^+	A_g^+	A^+	A^+
Q_{4a}, Q_{4b}	G_{3a}, G_{3b}	A''^+	B^+	A_g^-	A^-	A^-
Q_{yz}, Q_{4v}^α	G_x, G_{3u}	E''	E_1	E_g	E	E
Q_{zx}, Q_{4u}^α	G_y, G_{3v}					
$Q_v, Q_{4u}^{\beta 1}, Q_{4u}^{\beta 2}$	G_{xyz}	E'	E_2	E_g	E	E
$Q_{xy}, Q_{4v}^{\beta 1}, Q_{4v}^{\beta 2}$	G_z^β					
Q_z, Q_z^α	G_0, G_u, G_{40}	A''^-	A^-	A_u^+	A^-	A^+
Q_{3a}, Q_{3b}	G_{4a}, G_{4b}	A'^-	B^-	A_u^-	A^+	A^-
Q_x, Q_{3u}	G_{yz}, G_{4v}^α	E'	E_1	E_u	E	E
Q_y, Q_{3v}	G_{zx}, G_{4u}^α					
Q_{xyz}	$G_v, G_{4u}^{\beta 1}, G_{4u}^{\beta 2}$	E''	E_2	E_u	E	E
Q_z^β	$G_{xy}, G_{4v}^{\beta 1}, G_{4v}^{\beta 2}$					
MT	M					
T_0, T_u, T_{40}	M_z, M_z^α	A'^-	A^-	A_g^-	A^-	A^-
T_{4a}, T_{4b}	M_{3a}, M_{3b}	A''^-	B^-	A_g^+	A^+	A^+
T_{yz}, T_{4v}^α	M_x, M_{3u}	E''	E_1	E_g	E	E
T_{zx}, T_{4u}^α	M_y, M_{3v}					
$T_v, T_{4u}^{\beta 1}, T_{4u}^{\beta 2}$	M_{xyz}	E'	E_2	E_g	E	E
$T_{xy}, T_{4v}^{\beta 1}, T_{4v}^{\beta 2}$	M_z^β					
T_z, T_z^α	M_0, M_u, M_{40}	A''^+	A^+	A_u^-	A^+	A^-
T_{3a}, T_{3b}	M_{4a}, M_{4b}	A'^+	B^+	A_u^+	A^-	A^+
T_x, T_{3u}	M_{yz}, M_{4v}^α	E'	E_1	E_u	E	E
T_y, T_{3v}	M_{zx}, M_{4u}^α					
T_{xyz}	$M_v, M_{4u}^{\beta 1}, M_{4u}^{\beta 2}$	E''	E_2	E_u	E	E
T_z^β	$M_{xy}, M_{4v}^{\beta 1}, M_{4v}^{\beta 2}$					

$$\begin{aligned}
 Y_{xyz} &= \chi_{xyz}^{O(1 \times 2)}, \quad Y_x^\alpha = \frac{1}{20} \left(5\chi_{xxx}^{O(1 \times 2)} - 3 \sum_i \chi_{xii}^{O(1 \times 2)} \right), \quad Y_y^\alpha = \frac{1}{20} \left(5\chi_{yyy}^{O(1 \times 2)} - 3 \sum_i \chi_{yii}^{O(1 \times 2)} \right), \\
 Y_z^\alpha &= \frac{1}{20} \left(5\chi_{zzz}^{O(1 \times 2)} - 3 \sum_i \chi_{zii}^{O(1 \times 2)} \right), \quad Y_x^\beta = \frac{1}{4} (\chi_{xyy}^{O(1 \times 2)} - \chi_{zzx}^{O(1 \times 2)}), \quad Y_y^\beta = \frac{1}{4} (\chi_{yzz}^{O(1 \times 2)} - \chi_{xxy}^{O(1 \times 2)}), \quad Y_z^\beta = \frac{1}{4} (\chi_{zxx}^{O(1 \times 2)} - \chi_{yyz}^{O(1 \times 2)}).
 \end{aligned}
 \tag{F16}$$

We set

$$(\tilde{X}_x, \tilde{X}'_x) \equiv (X'_x - 4X_x, X'_x + 2X_x), \text{ (cyclic)}, \tag{F17}$$

for notational simplicity.

4. $\chi^{[0 \times 3]}$

The multipoles in Eq. (23) are represented by using $\chi_{0;ijk}^{[0 \times 3]}$, which is totally symmetric for the permutation of i, j , and k as follows:

$$\begin{aligned}
 (X_x, X_y, X_z) &= \frac{1}{5} \left(\sum_i \chi_{0;xii}^{[0 \times 3]}, \sum_i \chi_{0;yii}^{[0 \times 3]}, \sum_i \chi_{0;zii}^{[0 \times 3]} \right), \\
 X_{xyz} &= \chi_{0;xyz}^{[0 \times 3]}, \quad X_x^\alpha = \frac{1}{10} \left(5\chi_{0;xxx}^{[0 \times 3]} - 3 \sum_i \chi_{0;xii}^{[0 \times 3]} \right), \quad X_y^\alpha = \frac{1}{10} \left(5\chi_{0;yyy}^{[0 \times 3]} - 3 \sum_i \chi_{0;yii}^{[0 \times 3]} \right),
 \end{aligned}
 \tag{F18}$$

TABLE XXXIV. IRREPs of multipoles in trigonal black-and-white point groups. $\{X_y - iX_x, X_y + iX_x\}$, $\{X_{zx} + iX_{yz}, X_{zx} - iX_{yz}\}$, $\{X_v - iX_{xy}, X_v + iX_{xy}\}$, $\{X_{3v} - iX_{3u}, X_{3v} + iX_{3u}\}$, $\{X_{xyz} + iX_z^\beta, X_{xyz} - iX_z^\beta\}$, $\{X_{4u}^\alpha + iX_{4v}^\alpha, X_{4u}^\alpha - iX_{4v}^\alpha\}$, $\{X_{4u}^{\beta 1} + iX_{4v}^{\beta 1}, X_{4u}^{\beta 1} - iX_{4v}^{\beta 1}\}$, and $\{X_{4u}^{\beta 2} - iX_{4v}^{\beta 2}, X_{4u}^{\beta 2} + iX_{4v}^{\beta 2}\}$ ($X = Q, G, T, M$) are the basis of $E_{g/u}^{(1,2)\pm}$ in $\bar{3}m'$ and $E^{(1,2)\pm}$ in $32'$ and $3m'$.

Magnetic point group	$\bar{3}m'$	$\bar{3}m$	$\bar{3}m'$	$32'$	$3m'$	$\bar{3}'$
Unitary subgroup	32	3m	$\bar{3}$	3	3	3
Antiuunitary operation	θI	θI	$\theta C'_2$	$\theta C'_2$	$\theta \sigma_v$	θI
E	ET					
Q_0, Q_u, Q_{40}, Q_{4b}	G_{3b}	A_1^+	A_1^+	A_g^+	A^+	A^+
Q_{4a}	G_z, G_z^α, G_{3a}	A_2^+	A_2^+	A_g^-	A^-	A^+
$Q_{yz}, Q_{xy}, Q_{4v}^\alpha, Q_{4v}^{\beta 1}, Q_{4v}^{\beta 2}$	G_x, G_{3u}, G_z^β	E^+	E^+	$E_g^{(1,2)+}$	$E^{(1,2)+}$	$E^{(1,2)+}$
$Q_{zx}, Q_v, Q_{4u}^\alpha, Q_{4u}^{\beta 1}, Q_{4u}^{\beta 2}$	G_y, G_{3v}, G_{xyz}					
Q_{3b}	G_0, G_u, G_{40}, G_{4b}	A_1^-	A_2^-	A_u^+	A^+	A^-
Q_z, Q_z^α, Q_{3a}	G_{4a}	A_2^-	A_1^-	A_u^-	A^-	A^-
Q_x, Q_{3u}, Q_z^β	$G_{yz}, G_{xy}, G_{4v}^\alpha, G_{4v}^{\beta 1}, G_{4v}^{\beta 2}$	E^-	E^-	$E_u^{(1,2)+}$	$E^{(1,2)+}$	$E^{(1,2)-}$
Q_y, Q_{3v}, Q_{xyz}	$G_{zx}, G_v, G_{4u}^\alpha, G_{4u}^{\beta 1}, G_{4u}^{\beta 2}$					
MT	M					
T_0, T_u, T_{40}, T_{4b}	M_{3b}	A_1^-	A_1^-	A_g^-	A^-	A^-
T_{4a}	M_z, M_z^α, M_{3a}	A_2^-	A_2^-	A_g^+	A^+	A^-
$T_{yz}, T_{xy}, T_{4v}^\alpha, T_{4v}^{\beta 1}, T_{4v}^{\beta 2}$	M_x, M_{3u}, M_z^β	E^-	E^-	$E_g^{(1,2)-}$	$E^{(1,2)-}$	$E^{(1,2)-}$
$T_{zx}, T_v, T_{4u}^\alpha, T_{4u}^{\beta 1}, T_{4u}^{\beta 2}$	M_y, M_{3v}, M_{xyz}					
T_{3b}	M_0, M_u, M_{40}, M_{4b}	A_1^+	A_2^+	A_u^-	A^-	A^+
T_z, T_z^α, T_{3a}	M_{4a}	A_2^+	A_1^+	A_u^+	A^+	A^+
T_x, T_{3u}, T_z^β	$M_{yz}, M_{xy}, M_{4v}^\alpha, M_{4v}^{\beta 1}, M_{4v}^{\beta 2}$	E^+	E^+	$E_u^{(1,2)-}$	$E^{(1,2)-}$	$E^{(1,2)+}$
T_y, T_{3v}, T_{xyz}	$M_{zx}, M_v, M_{4u}^\alpha, M_{4u}^{\beta 1}, M_{4u}^{\beta 2}$					

$$X_z^\alpha = \frac{1}{10} \left(5\chi_{0;zzz}^{[0\times 3]} - 3 \sum_i \chi_{0;zii}^{[0\times 3]} \right), \quad X_x^\beta = \frac{1}{2} (\chi_{0;xyy}^{[0\times 3]} - \chi_{0;zzx}^{[0\times 3]}), \quad X_y^\beta = \frac{1}{2} (\chi_{0;yzx}^{[0\times 3]} - \chi_{0;xyx}^{[0\times 3]}), \quad X_z^\beta = \frac{1}{2} (\chi_{0;zzx}^{[0\times 3]} - \chi_{0;yyz}^{[0\times 3]}). \quad (F19)$$

5. $\chi^{[1\times 3]}$

The monopole, dipole, quadrupole, octupole, and hexadecapole components of $\chi^{[1\times 3]}$ are represented by using $\chi_{i;jkl}^{[1\times 3]}$, which is totally symmetric by the permutation of j, k , and l , as

$$\chi^{M(1\times 1)} = \frac{1}{3} \sum_{ij} \chi_{i;ijj}^{[1\times 3]}, \quad (F20)$$

$$\chi_i^{D(1\times 1)} = \frac{1}{2} \sum_{jkl} \epsilon_{ijk} \chi_{j;klj}^{[1\times 3]}, \quad (F21)$$

$$\chi_{ij}^{Q(1\times 1)} = \frac{1}{6} \sum_k (\chi_{i;jkk}^{[1\times 3]} + \chi_{j;ikk}^{[1\times 3]}) = \chi_{ji}^{Q(1\times 1)}, \quad (F22)$$

$$\chi_{ij}^{Q(1\times 3)} = \frac{1}{2} \sum_k \left[(\chi_{k;ijk}^{[1\times 3]} + \chi_{k;jik}^{[1\times 3]}) - \frac{2}{5} (\chi_{i;jkk}^{[1\times 3]} + \chi_{j;ikk}^{[1\times 3]}) \right] = \chi_{ji}^{Q(1\times 3)}, \quad (F23)$$

$$\chi_{ijk}^{O(1\times 3)} = \frac{1}{6} \sum_{lm} (\epsilon_{klm} \chi_{l;ijm}^{[1\times 3]} + \epsilon_{ilm} \chi_{l;jkm}^{[1\times 3]} + \epsilon_{jlm} \chi_{l;kim}^{[1\times 3]}) = \chi_{jki}^{O(1\times 3)} = \chi_{jik}^{O(1\times 3)}, \quad (F24)$$

$$\chi_{ijkl}^{H(1\times 3)} = \frac{1}{4} (\chi_{i;jkl}^{[1\times 3]} + \chi_{j;kli}^{[1\times 3]} + \chi_{k;lij}^{[1\times 3]} + \chi_{l;jik}^{[1\times 3]}) = \chi_{jkli}^{H(1\times 3)} = \chi_{jikl}^{H(1\times 3)}. \quad (F25)$$

The field $F^{[3]} = (F_{xxx}, F_{yyy}, F_{zzz}, F_{yyz}, F_{zzx}, F_{xxy}, F_{yzx}, F_{zxx}, F_{xyy}, F_{xyz})$ is decomposed into the $I_F = 1$ and 3 components. The $I_F = 1$ field in $F^{[3]}$ leads to the monopole, dipole, and quadrupole components, $\chi^{M(1\times 1)}$, $\chi^{D(1\times 1)}$, and $\chi^{Q(1\times 1)}$, whereas the $I_F = 3$ field in $F^{[3]}$ results in the quadrupole, octupole, and hexadecapole components, $\chi^{Q(1\times 3)}$, $\chi^{O(1\times 3)}$, and $\chi^{H(1\times 3)}$.

TABLE XXXV. Laue group (LG) and the corresponding three types of magnetic point groups: gray point group (GPG), crystallographic point group (CPG), and black-and-white point group (BWPG).

LG	GPG	CPG	BWPG
$m\bar{3}m$	$m\bar{3}m1'$ 4321'	$m\bar{3}m$ 432	$m'\bar{3}'m'$, $m\bar{3}m'$, $m'\bar{3}'m$ 4'32'
$m\bar{3}$	$\bar{4}3m1'$ $m\bar{3}1'$ 231'	$\bar{4}3m$ $m\bar{3}$ 23	$\bar{4}'3m'$ $\bar{m}'\bar{3}'$
$4/mmm$	$4/mmm1'$ 4221' $\bar{4}2m1'$ $4mm1'$	$4/mmm$ 422 $\bar{4}2m$ $4mm$	$4/m'm'm'$, $4/mm'm'$ $4'/m'm'm$, $4'/mm'm$, $4/m'mmm$ 42'2', 4'22' $\bar{4}2'm'$, $\bar{4}'2m'$, $\bar{4}'2'm$ $4m'm'$, $4'm'm$
$4/m$	$4/m1'$ 41' $\bar{4}1'$	$4/m$ 4 $\bar{4}$	$4'/m'$, $4/m'$, $4'/m$ 4' $\bar{4}$
mmm	$mmm1'$ 2221' $mm21'$	mmm 222 $mm2$	$m'm'm'$, $m'm'm$, $m'mm$ 2'2'2 $m'm'2$, $m'm2'$
$2/m$	$2/m1'$ 21' $m1'$	$2/m$ 2 m	$2'/m'$, $2/m'$, $2'/m$ 2' m'
$\bar{1}$	$\bar{1}1'$ 11'	$\bar{1}$ 1	$\bar{1}'$
$6/mmm$	$6/mmm1'$ 6221' $\bar{6}m21'$ $6mm1'$	$6/mmm$ 622 $\bar{6}m2$ $6mm$	$6/m'm'm'$, $6/mm'm'$ $6'/m'mm'$, $6'/mmm'$, $6/m'mmm$ 62'2', 6'22' $\bar{6}m'2'$, $\bar{6}'m2'$, $\bar{6}'m'2$ $6m'm'$, $6'mm'$
$6/m$	$6/m1'$ 61' $\bar{6}1'$	$6/m$ 6 $\bar{6}$	$6'/m'$, $6/m'$, $6'/m$ 6' $\bar{6}'$
$\bar{3}m$	$\bar{3}m1'$ 321' $3m1'$	$\bar{3}m$ 32 $3m$	$\bar{3}m'$, $\bar{3}'m'$, $\bar{3}'m$ 32' $3m'$
$\bar{3}$	$\bar{3}1'$ 31'	$\bar{3}$ 3	$\bar{3}'$

By using Eqs. (F20)–(F25), the multipoles in Eq. (24) are shown as

$$X_0 = \frac{1}{5} \chi^{M(1 \times 1)}, \quad (F26)$$

$$Y_x = \frac{1}{5} \chi_x^{D(1 \times 1)}, \quad Y_y = \frac{1}{5} \chi_y^{D(1 \times 1)}, \quad Y_z = \frac{1}{5} \chi_z^{D(1 \times 1)}, \quad (F27)$$

$$X_u = \frac{1}{42} \left(3\chi_{zz}^{Q(1 \times 3)} - \sum_i \chi_{ii}^{Q(1 \times 3)} \right), \quad X_v = \frac{1}{42} (\chi_{xx}^{Q(1 \times 3)} - \chi_{yy}^{Q(1 \times 3)}), \quad X_{yz} = \frac{1}{21} \chi_{yz}^{Q(1 \times 3)},$$

$$X_{zx} = \frac{1}{21} \chi_{zx}^{Q(1 \times 3)}, \quad X_{xy} = \frac{1}{21} \chi_{xy}^{Q(1 \times 3)}, \quad (F28)$$

$$X'_u = \frac{1}{10} \left(3\chi_{zz}^{Q(1 \times 1)} - \sum_i \chi_{ii}^{Q(1 \times 1)} \right), \quad X'_v = \frac{3}{10} (\chi_{xx}^{Q(1 \times 1)} - \chi_{yy}^{Q(1 \times 1)}), \quad X'_{yz} = \frac{3}{5} \chi_{yz}^{Q(1 \times 1)}, \quad X'_{zx} = \frac{3}{5} \chi_{zx}^{Q(1 \times 1)}, \quad X'_{xy} = \frac{3}{5} \chi_{xy}^{Q(1 \times 1)}, \quad (F29)$$

TABLE XXXVI. Magnetic Laue group (MLG) for the gray point group (GPG) and the \mathcal{PT} -symmetric black-and-white point group (BWPG).

MLG	GPG	BWPG
$m\bar{3}m1'$	$m\bar{3}m1'$ 4321'	$m'\bar{3}'m', m'\bar{3}'m$
$m\bar{3}1'$	$\bar{4}3m1'$ $m\bar{3}1'$ 231'	$m'\bar{3}'$
$4/mmm1'$	$4/mmm1'$ 4221'	$4/m'm'm', 4'/m'm'm, 4/m'mm$
$4/m1'$	$\bar{4}2m1'$ $4mm1'$ $4/m1'$ 41' $\bar{4}1'$	$4'/m', 4/m'$
$mmm1'$	$mmm1'$ 2221'	$m'm'm', m'mm$
$2/m1'$	$mm21'$ $2/m1'$ 21' $m1'$ $\bar{1}1'$ 11'	$2'/m, 2/m'$
$\bar{1}1'$	$\bar{1}1'$ 11'	$\bar{1}'$
$6/mmm1'$	$6/mmm1'$ 6221'	$6/m'm'm', 6'/mmm', 6/m'mm$
$6/m1'$	$\bar{6}m21'$ $6mm1'$ $6/m1'$ 61' $\bar{6}1'$	$6'/m, 6/m'$
$\bar{3}m1'$	$\bar{3}m1'$ 321'	$\bar{3}'m', \bar{3}'m$
$\bar{3}1'$	$3m1'$ $\bar{3}1'$ 31'	$\bar{3}'$

$$\begin{aligned}
 Y_{xyz} &= \chi_{xyz}^{O(1 \times 3)}, \quad Y_x^\alpha = \frac{1}{20} \left(5\chi_{xxx}^{O(1 \times 3)} - 3 \sum_i \chi_{xii}^{O(1 \times 3)} \right), \quad Y_y^\alpha = \frac{1}{20} \left(5\chi_{yyy}^{O(1 \times 3)} - 3 \sum_i \chi_{yii}^{O(1 \times 3)} \right), \\
 Y_z^\alpha &= \frac{1}{20} \left(5\chi_{zzz}^{O(1 \times 3)} - 3 \sum_i \chi_{zii}^{O(1 \times 3)} \right), \quad Y_x^\beta = \frac{1}{4} (\chi_{xyy}^{O(1 \times 3)} - \chi_{zzx}^{O(1 \times 3)}), \\
 Y_y^\beta &= \frac{1}{4} (\chi_{yzz}^{O(1 \times 3)} - \chi_{xxy}^{O(1 \times 3)}), \quad Y_z^\beta = \frac{1}{4} (\chi_{zxx}^{O(1 \times 3)} - \chi_{yyz}^{O(1 \times 3)}),
 \end{aligned} \tag{F30}$$

$$\begin{aligned}
 X_4 &= \frac{1}{15} \left[\sum_i \chi_{iiii}^{H(1 \times 3)} - 3(\chi_{yyzz}^{H(1 \times 3)} + \chi_{zzxx}^{H(1 \times 3)} + \chi_{xxyy}^{H(1 \times 3)}) \right], \\
 X_{4u} &= \frac{1}{42} \left[3\chi_{zzzz}^{H(1 \times 3)} - \sum_i \chi_{iiii}^{H(1 \times 3)} + 6(2\chi_{xxyy}^{H(1 \times 3)} - \chi_{yyzz}^{H(1 \times 3)} - \chi_{zzxx}^{H(1 \times 3)}) \right], \\
 X_{4v} &= \frac{1}{14} [\chi_{xxxx}^{H(1 \times 3)} - \chi_{yyyy}^{H(1 \times 3)} + 6(\chi_{yyzz}^{H(1 \times 3)} - \chi_{zzxx}^{H(1 \times 3)})], \quad X_{4x}^\alpha = \frac{1}{2} (\chi_{yyyz}^{H(1 \times 3)} - \chi_{yzzz}^{H(1 \times 3)}), \quad X_{4y}^\alpha = \frac{1}{2} (\chi_{zzzx}^{H(1 \times 3)} - \chi_{zzxx}^{H(1 \times 3)}), \\
 X_{4z}^\alpha &= \frac{1}{2} (\chi_{xxyy}^{H(1 \times 3)} - \chi_{xyyy}^{H(1 \times 3)}), \quad X_{4x}^\beta = \frac{1}{14} \left(7\chi_{xxyz}^{H(1 \times 3)} - \sum_i \chi_{iizy}^{H(1 \times 3)} \right),
 \end{aligned}$$

TABLE XXXVII. Magnetic Laue group (MLG) for the crystallographic point group (CPG) and the \mathcal{PT} -breaking black-and-white point group (BWPG).

MLG	CPG	MLG	BWPG
$m\bar{3}m$	$m\bar{3}m$ 432 $\bar{4}3m$	$m\bar{3}m'$	$m\bar{3}m'$ $4'32'$ $\bar{4}'3m'$
$m\bar{3}$	$m\bar{3}$ 23	$4/mmm'$	$4/mmm'$ $42'2'$ $\bar{4}2'm'$
$4/mmm$	$4/mmm$ 422 $\bar{4}2m$	$4'/mm'm$	$4m'm'$ $4'/mm'm$ $4'22'$
$4/m$	$4/m$ 4 $\bar{4}$	$4'/m$	$\bar{4}'2m', \bar{4}'2'm$ $4'm'm$ $4'/m$
mmm	mmm 222 $mm2$	$m'm'm$	$4'$ $\bar{4}'$ $m'm'm$ $2'2'2$
$2/m$	$2/m$ 2 m	$2'/m'$	$m'm'2, m'm2'$ $2'/m'$ $2'$ m'
$\bar{1}$	$\bar{1}$ 1		m'
$6/mmm$	$6/mmm$ 622 $\bar{6}m2$ $6mm$	$6/mmm'$	$6/mmm'$ $62'2'$ $\bar{6}m'2'$ $6m'm'$
$6/m$	$6/m$ 6 $\bar{6}$	$6'/m'mm'$	$6'/m'mm'$ $6'22'$ $\bar{6}'m2', \bar{6}'m'2$
$\bar{3}m$	$\bar{3}m$ 32 $3m$	$6'/m'$	$6'mm'$ $6'/m'$ $6'$ $\bar{6}'$
$\bar{3}$	$\bar{3}$ 3	$\bar{3}m'$	$\bar{3}m'$ $32'$ $3m'$

$$X_{4y}^\beta = \frac{1}{14} \left(7\chi_{yyzx}^{H(1 \times 3)} - \sum_i \chi_{iizx}^{H(1 \times 3)} \right), \quad X_{4z}^\beta = \frac{1}{14} \left(7\chi_{zzxy}^{H(1 \times 3)} - \sum_i \chi_{iixy}^{H(1 \times 3)} \right). \quad (\text{F31})$$

For notational simplicity, we take

$$\begin{aligned} (\tilde{X}_u, \tilde{X}'_u) &\equiv (X_u + X'_u, 4X_u - X'_u), \quad \tilde{X}''_u \equiv \tilde{X}_u - \tilde{X}'_u, \quad (\tilde{X}_v, \tilde{X}'_v) \equiv (3X_v + X'_v, 2X_v - X'_v), \quad \tilde{X}''_v \equiv \tilde{X}_v + 2\tilde{X}'_v, \\ (\tilde{X}_{yz}, \tilde{X}'_{yz}) &\equiv (2X_{yz} - X'_{yz}, 8X_{yz} + X'_{yz}), \quad (\text{cyclic}). \end{aligned} \quad (\text{F32})$$

6. $\chi^{[2 \times 2]}$

For the rank-4 tensor $\chi^{[2 \times 2]}$,

$$\chi^{[2 \times 2]} = \begin{pmatrix} \chi_{ll} & \chi_{lt} \\ \chi_{tl} & \chi_{tt} \end{pmatrix}, \quad (\text{F33})$$

$$\begin{aligned} \chi_{ll} &= \begin{pmatrix} \chi_{xx;xx}^{[2 \times 2]} & \chi_{xx;yy}^{[2 \times 2]} & \chi_{xx;zz}^{[2 \times 2]} \\ \chi_{yy;xx}^{[2 \times 2]} & \chi_{yy;yy}^{[2 \times 2]} & \chi_{yy;zz}^{[2 \times 2]} \\ \chi_{zz;xx}^{[2 \times 2]} & \chi_{zz;yy}^{[2 \times 2]} & \chi_{zz;zz}^{[2 \times 2]} \end{pmatrix}, & \chi_{lt} &= \begin{pmatrix} \chi_{xx;yz}^{[2 \times 2]} & \chi_{xx;zx}^{[2 \times 2]} & \chi_{xx;xy}^{[2 \times 2]} \\ \chi_{yy;yz}^{[2 \times 2]} & \chi_{yy;zx}^{[2 \times 2]} & \chi_{yy;xy}^{[2 \times 2]} \\ \chi_{zz;yz}^{[2 \times 2]} & \chi_{zz;zx}^{[2 \times 2]} & \chi_{zz;xy}^{[2 \times 2]} \end{pmatrix}, \\ \chi_{tl} &= \begin{pmatrix} \chi_{yz;xx}^{[2 \times 2]} & \chi_{yz;yy}^{[2 \times 2]} & \chi_{yz;zz}^{[2 \times 2]} \\ \chi_{zx;xx}^{[2 \times 2]} & \chi_{zx;yy}^{[2 \times 2]} & \chi_{zx;zz}^{[2 \times 2]} \\ \chi_{xy;xx}^{[2 \times 2]} & \chi_{xy;yy}^{[2 \times 2]} & \chi_{xy;zz}^{[2 \times 2]} \end{pmatrix}, & \chi_{tt} &= \begin{pmatrix} \chi_{yz;yz}^{[2 \times 2]} & \chi_{yz;zx}^{[2 \times 2]} & \chi_{yz;xy}^{[2 \times 2]} \\ \chi_{zx;yz}^{[2 \times 2]} & \chi_{zx;zx}^{[2 \times 2]} & \chi_{zx;xy}^{[2 \times 2]} \\ \chi_{xy;yz}^{[2 \times 2]} & \chi_{xy;zx}^{[2 \times 2]} & \chi_{xy;xy}^{[2 \times 2]} \end{pmatrix}, \end{aligned} \quad (\text{F34})$$

the monopole, dipole, quadrupole, octupole, and hexadecapole components are expressed by using the tensor component $\chi_{ij;kl}^{[2 \times 2]}$ ($= \chi_{ji;kl}^{[2 \times 2]} = \chi_{ij;lk}^{[2 \times 2]}$) as

$$\chi^{M(0 \times 0)} = \frac{1}{3} \sum_{ij} \chi_{ii;jj}^{[2 \times 2]}, \quad (\text{F35})$$

$$\chi_{ij}^{Q(0 \times 2, \pm)} = \frac{1}{6} \sum_k (\chi_{kk;ij}^{[2 \times 2]} \pm \chi_{ij;kk}^{[2 \times 2]}), \quad (\text{F36})$$

$$\chi^{M(2 \times 2)} = \frac{1}{3} \sum_{ij} \left(\chi_{ij;ji}^{[2 \times 2]} - \frac{1}{3} \chi_{ii;jj}^{[2 \times 2]} \right), \quad (\text{F37})$$

$$\chi_i^{D(2 \times 2)} = \frac{1}{2} \sum_{jkl} \epsilon_{ijk} \chi_{lj;kl}^{[2 \times 2]}, \quad (\text{F38})$$

$$\chi_{ij}^{Q(2 \times 2)} = \frac{1}{2} \sum_k \left[(\chi_{ik;kj}^{[2 \times 2]} + \chi_{jk;ki}^{[2 \times 2]}) - \frac{2}{3} (\chi_{ij;kk}^{[2 \times 2]} + \chi_{kk;ij}^{[2 \times 2]}) \right] = \chi_{ji}^{Q(2 \times 2)}, \quad (\text{F39})$$

$$\chi_{ijk}^{O(2 \times 2)} = \frac{1}{6} \sum_{lm} (\epsilon_{ilm} \chi_{jl;mk}^{[2 \times 2]} + \epsilon_{jlm} \chi_{kl;mi}^{[2 \times 2]} + \epsilon_{klm} \chi_{il;mj}^{[2 \times 2]} + \epsilon_{ilm} \chi_{kl;mj}^{[2 \times 2]} + \epsilon_{jlm} \chi_{il;mk}^{[2 \times 2]} + \epsilon_{klm} \chi_{jl;mi}^{[2 \times 2]}) = \chi_{jki}^{O(2 \times 2)} = \chi_{jik}^{O(2 \times 2)}, \quad (\text{F40})$$

$$\chi_{ijkl}^{H(2 \times 2)} = \frac{1}{6} (\chi_{ij;kl}^{[2 \times 2]} + \chi_{ik;jl}^{[2 \times 2]} + \chi_{il;kj}^{[2 \times 2]} + \chi_{kj;il}^{[2 \times 2]} + \chi_{lj;ki}^{[2 \times 2]} + \chi_{kl;ij}^{[2 \times 2]}) = \chi_{jkli}^{H(2 \times 2)} = \chi_{jikl}^{H(2 \times 2)}. \quad (\text{F41})$$

Since both $B^{[2]} = (B_{xx}, B_{yy}, B_{zz}, B_{yz}, B_{zx}, B_{xy})$ and $F^{[2]} = (F_{xx}, F_{yy}, F_{zz}, F_{yz}, F_{zx}, F_{xy})$ contain $l_B, l_F = 0$ and 2 components, there are two types of monopole components $\chi^{M(0 \times 0)}$ and $\chi^{M(2 \times 2)}$ and three types of quadrupole component $\chi_{ij}^{Q(0 \times 2, \pm)}$ and $\chi_{ij}^{Q(2 \times 2)}$. By using Eqs. (F35)–(F41), the multipoles in Eqs. (26)–(29) are represented by

$$X_0 = \frac{1}{10} \chi^{M(2 \times 2)}, \quad X'_0 = \frac{1}{3} \chi^{M(0 \times 0)}, \quad (\text{F42})$$

$$Y_x = \frac{1}{5} \chi_x^{D(2 \times 2)}, \quad Y_y = \frac{1}{5} \chi_y^{D(2 \times 2)}, \quad Y_z = \frac{1}{5} \chi_z^{D(2 \times 2)}, \quad (\text{F43})$$

$$\begin{aligned} X_u &= \frac{1}{42} \left(3 \chi_{zz}^{Q(2 \times 2)} - \sum_i \chi_{ii}^{Q(2 \times 2)} \right), & X_v &= \frac{1}{14} (\chi_{xx}^{Q(2 \times 2)} - \chi_{yy}^{Q(2 \times 2)}), & X_{yz} &= \frac{1}{7} \chi_{yz}^{Q(2 \times 2)}, \\ X_{zx} &= \frac{1}{7} \chi_{zx}^{Q(2 \times 2)}, & X_{xy} &= \frac{1}{7} \chi_{xy}^{Q(2 \times 2)}, \end{aligned} \quad (\text{F44})$$

$$\begin{aligned} X_u^{(\pm)} &= \frac{1}{6} \left(3 \chi_{zz}^{Q(0 \times 2, \pm)} - \sum_i \chi_{ii}^{Q(0 \times 2, \pm)} \right), & X_v^{(\pm)} &= \frac{1}{2} (\chi_{xx}^{Q(0 \times 2, \pm)} - \chi_{yy}^{Q(0 \times 2, \pm)}), & X_{yz}^{(\pm)} &= \chi_{yz}^{Q(0 \times 2, \pm)}, \\ X_{zx}^{(\pm)} &= \chi_{zx}^{Q(0 \times 2, \pm)}, & X_{xy}^{(\pm)} &= \chi_{xy}^{Q(0 \times 2, \pm)}, \end{aligned} \quad (\text{F45})$$

$$\begin{aligned} Y_{xyz} &= \chi_{xyz}^{O(2 \times 2)}, \\ Y_x^\alpha &= \frac{1}{20} \left(5 \chi_{xxx}^{O(2 \times 2)} - 3 \sum_i \chi_{xii}^{O(2 \times 2)} \right), & Y_y^\alpha &= \frac{1}{20} \left(5 \chi_{yyy}^{O(2 \times 2)} - 3 \sum_i \chi_{yii}^{O(2 \times 2)} \right), & Y_z^\alpha &= \frac{1}{20} \left(5 \chi_{zzz}^{O(2 \times 2)} - 3 \sum_i \chi_{zii}^{O(2 \times 2)} \right), \\ Y_x^\beta &= \frac{1}{4} (\chi_{xyy}^{O(2 \times 2)} - \chi_{zxx}^{O(2 \times 2)}), & Y_y^\beta &= \frac{1}{4} (\chi_{yzz}^{O(2 \times 2)} - \chi_{xxy}^{O(2 \times 2)}), & Y_z^\beta &= \frac{1}{4} (\chi_{zxx}^{O(2 \times 2)} - \chi_{yyz}^{O(2 \times 2)}), \end{aligned} \quad (\text{F46})$$

$$X_4 = \frac{1}{6} \left(\sum_i \chi_{iiii}^{H(2 \times 2)} - \frac{3}{5} \sum_{ij} \chi_{iijj}^{H(2 \times 2)} \right), \quad X_{4u} = \frac{1}{6} \left[\left(3 \chi_{zzzz}^{H(2 \times 2)} - \sum_i \chi_{iiii}^{H(2 \times 2)} \right) - \frac{6}{7} \sum_i (2 \chi_{iizz}^{H(2 \times 2)} - \chi_{iixx}^{H(2 \times 2)} - \chi_{iyyy}^{H(2 \times 2)}) \right],$$

$$\begin{aligned}
 X_{4v} &= \frac{1}{2} \left[\chi_{xxxx}^{\text{H}(2 \times 2)} - \chi_{yyyy}^{\text{H}(2 \times 2)} - \frac{6}{7} \sum_i (\chi_{iixx}^{\text{H}(2 \times 2)} - \chi_{iyyy}^{\text{H}(2 \times 2)}) \right], & X_{4x}^\alpha &= \frac{1}{2} (\chi_{yyyz}^{\text{H}(2 \times 2)} - \chi_{yzzz}^{\text{H}(2 \times 2)}), & X_{4y}^\alpha &= \frac{1}{2} (\chi_{zzzx}^{\text{H}(2 \times 2)} - \chi_{zzxx}^{\text{H}(2 \times 2)}), \\
 X_{4z}^\alpha &= \frac{1}{2} (\chi_{xxyy}^{\text{H}(2 \times 2)} - \chi_{xyyy}^{\text{H}(2 \times 2)}), & X_{4x}^\beta &= \frac{1}{2} \left(6\chi_{xxyz}^{\text{H}(2 \times 2)} - \frac{1}{7} \sum_i \chi_{yzi}^{\text{H}(2 \times 2)} \right), & X_{4y}^\beta &= \frac{1}{2} \left(6\chi_{yyzx}^{\text{H}(2 \times 2)} - \frac{1}{7} \sum_i \chi_{zxi}^{\text{H}(2 \times 2)} \right), \\
 X_{4z}^\beta &= \frac{1}{2} \left(6\chi_{zzxy}^{\text{H}(2 \times 2)} - \frac{1}{7} \sum_i \chi_{xyii}^{\text{H}(2 \times 2)} \right). & & & &
 \end{aligned} \tag{F47}$$

We use the notation

$$\begin{aligned}
 (\tilde{X}_0, \tilde{X}'_0) &\equiv (4X_0 + X'_0, -2X_0 + X'_0), & (\tilde{X}_u, \tilde{X}_u^{(\pm)}) &\equiv (-4X_u - 2X_u^{(+)}, -4X_u + X_u^{(+)} \pm 3X_u^{(-)}), & \tilde{X}'_u &\equiv -\tilde{X}_u^{(+)} - \tilde{X}_u^{(-)}, \\
 (\tilde{X}_v, \tilde{X}_v^{(\pm)}) &\equiv (4X_v + 2X_v^{(+)}, -4X_v + X_v^{(+)} \pm X_v^{(-)}), & (\tilde{X}'_{yz}, \tilde{X}'_{yz}^{(\pm)}) &\equiv (-4X_{yz} + X_{yz}^{(+)} \pm X_{yz}^{(-)}, 2X_{yz} + X_{yz}^{(+)} \pm X_{yz}^{(-)}), & & \text{(cyclic)},
 \end{aligned} \tag{F48}$$

for simplicity.

APPENDIX G: TENSOR EXPRESSION IN HEXAGONAL/TRIGONAL SYSTEM

In the hexagonal and trigonal systems, multipoles are expressed by the tesseral harmonics. Since the tesseral harmonics have the different functional form from the cubic harmonics for rank $l \geq 3$, we show the response tensors in the hexagonal and trigonal systems with rank $l \geq 3$ multipoles. The corresponding rank-3 and -4 tensors are represented by

$$\chi^{[0 \times 3]} = \begin{pmatrix} 3X_x + X_{3a} - 3X_{3u} \\ 3X_y - X_{3b} - 3X_{3v} \\ 3X_z + 2X_z^\alpha \\ X_z - X_z^\alpha - X_z^\beta \\ X_x + 4X_{3u} \\ X_y + X_{3b} - X_{3v} \\ X_y + 4X_{3v} \\ X_z - X_z^\alpha + X_z^\beta \\ X_x - X_{3a} - X_{3u} \\ X_{xyz} \end{pmatrix}^T, \tag{G1}$$

$$\chi^{[1 \times 2]} = \begin{pmatrix} \tilde{X}_x + X_{3a} - 3X_{3u} & \tilde{X}'_y - 2Y_{zx} + X_{3b} - X_{3v} & \tilde{X}'_z + 2Y_{xy} - 2X_z^\alpha + 2X_z^\beta \\ \tilde{X}'_x + 2Y_{yz} - X_{3a} - X_{3u} & \tilde{X}_y - X_{3b} - 3X_{3v} & \tilde{X}'_z - 2Y_{xy} - 2X_z^\alpha - 2X_z^\beta \\ \tilde{X}'_x - 2Y_{yz} + 4X_{3u} & \tilde{X}'_y + 2Y_{zx} + 4X_{3v} & \tilde{X}_z + 4X_z^\alpha \\ Y_u + Y_v + X_{xyz} & -3X_z + Y_{xy} - 2X_z^\alpha - 2X_z^\beta & -3X_y - Y_{zx} + 4X_{3v} \\ -3X_z - Y_{xy} - 2X_z^\alpha + 2X_z^\beta & -Y_u + Y_v + X_{xyz} & -3X_x + Y_{yz} + 4X_{3u} \\ -3X_y + Y_{zx} + X_{3b} - X_{3v} & -3X_x - Y_{yz} - X_{3a} - X_{3u} & -2Y_v + X_{xyz} \end{pmatrix}^T, \tag{G2}$$

$$\chi^{[1 \times 3]} = \begin{pmatrix} 3(X_0 - \tilde{X}_u + \tilde{X}_v) + 3X_{40} + X_{4u}^{\beta 1} - X_{4u}^{\beta 2} & 3(-Y_z - \tilde{X}_{xy} + Y_z^\alpha - Y_z^\beta) + X_{4v}^{\beta 1} - X_{4v}^{\beta 2} & 3(Y_y - \tilde{X}_{zx} + Y_{3b} - Y_{3v}) + X_{4b} - 3X_{4u}^\alpha \\ 3(Y_z - \tilde{X}_{xy} - Y_z^\alpha - Y_z^\beta) - X_{4v}^{\beta 1} - X_{4v}^{\beta 2} & 3(X_0 - \tilde{X}_u - \tilde{X}_v) + 3X_{40} + X_{4u}^{\beta 1} + X_{4u}^{\beta 2} & 3(-Y_x - \tilde{X}_{yz} + Y_{3a} + Y_{3u}) - X_{4a} - 3X_{4u}^\alpha \\ -3(Y_y + \tilde{X}_{zx} + 4Y_{3v}) + 4X_{4u}^\alpha & 3(Y_x - \tilde{X}_{yz} + 4Y_{3u}) + 4X_{4v}^\alpha & 3(X_0 + 2\tilde{X}_u) + 8X_{40} \\ -Y_y - \tilde{X}_{zx} + Y_{3b} + 11Y_{3v} - X_{4b} - X_{4u}^\alpha & Y_x + \tilde{X}'_{yz} - Y_{3a} - Y_{3u} - X_{4a} - 3X_{4v}^\alpha & X_0 + \tilde{X}''_u - 5X_v - Y_{xyz} - 4X_{40} - X_{4u}^{\beta 2} \\ X_0 + \tilde{X}'_u - \tilde{X}'_v - Y_{xyz} - 4X_{40} + X_{4u}^{\beta 2} & -Y_z - \tilde{X}_{xy} - 4Y_z^\alpha + 2Y_z^\beta + 2X_{4v}^{\beta 2} & Y_y + \tilde{X}'_{zx} + 4Y_{3v} + 4X_{4u}^\alpha \\ Y_z + \tilde{X}'_{xy} - Y_z^\alpha + Y_z^\beta + X_{4v}^{\beta 1} - X_{4v}^{\beta 2} & X_0 - \tilde{X}_u + \tilde{X}'_v - Y_{xyz} + X_{40} - X_{4u}^{\beta 1} & -Y_x - \tilde{X}'_{yz} - 3Y_{3a} + Y_{3u} + X_{4a} - X_{4v}^\alpha \\ Y_z - \tilde{X}_{xy} + 4Y_z^\alpha + 2Y_z^\beta + 2X_{4v}^{\beta 2} & X_0 + \tilde{X}'_u + \tilde{X}'_v + Y_{xyz} - 4X_{40} - X_{4u}^{\beta 2} & -Y_x + \tilde{X}'_{yz} - 4Y_{3u} + 4X_{4v}^\alpha \\ -Y_y + \tilde{X}'_{zx} - Y_{3b} + Y_{3v} + X_{4b} - 3X_{4u}^\alpha & Y_x - \tilde{X}'_{yz} + Y_{3a} - 11Y_{3u} + X_{4a} - X_{4v}^\alpha & X_0 + \tilde{X}''_u + 5X_v + Y_{xyz} - 4X_{40} + X_{4u}^{\beta 2} \\ X_0 - \tilde{X}_u - \tilde{X}'_v + Y_{xyz} + X_{40} - X_{4u}^{\beta 1} & -Y_z + \tilde{X}'_{xy} + Y_z^\alpha + Y_z^\beta - X_{4v}^{\beta 1} - X_{4v}^{\beta 2} & Y_y - \tilde{X}_{zx} - 3Y_{3b} - Y_{3v} - X_{4b} - X_{4u}^\alpha \\ 5X_{yz} + Y_{3a} + 5Y_{3u} + X_{4a} - X_{4v}^\alpha & 5X_{zx} + Y_{3b} - 5Y_{3v} - X_{4b} - X_{4u}^\alpha & 5X_{xy} - 2Y_z^\beta + 2X_{4v}^{\beta 2} \end{pmatrix}^T, \tag{G3}$$

$$\chi^{[2 \times 2]} = \begin{pmatrix} \chi_{ll} & \chi_{lt} \\ \chi_{tl} & \chi_{tt} \end{pmatrix}, \quad (G4)$$

$$\chi_{ll} = \begin{pmatrix} \tilde{X}'_0 + \tilde{X}'_u + \tilde{X}'_v + 3X_{40} + X_{4u}^{\beta 1} - X_{4u}^{\beta 2} & \tilde{X}'_0 + \tilde{X}'_u - 2\tilde{X}'_v + Y_{xyz} + X_{40} - X_{4u}^{\beta 1} & \tilde{X}'_0 + \tilde{X}'_u + \tilde{X}'_v - Y_{xyz} - 4X_{40} + X_{4u}^{\beta 2} \\ \tilde{X}'_0 + \tilde{X}'_u + 2\tilde{X}'_v - Y_{xyz} + X_{40} - X_{4u}^{\beta 1} & \tilde{X}'_0 + \tilde{X}'_u - \tilde{X}'_v + 3X_{40} + X_{4u}^{\beta 1} + X_{4u}^{\beta 2} & \tilde{X}'_0 + \tilde{X}'_u - \tilde{X}'_v + Y_{xyz} - 4X_{40} - X_{4u}^{\beta 2} \\ \tilde{X}'_0 + \tilde{X}'_u + \tilde{X}'_v + Y_{xyz} - 4X_{40} + X_{4u}^{\beta 2} & \tilde{X}'_0 + \tilde{X}'_u - \tilde{X}'_v - Y_{xyz} - 4X_{40} - X_{4u}^{\beta 2} & \tilde{X}'_0 - 2\tilde{X}'_u + 8X_{40} \end{pmatrix}, \quad (G5)$$

$$\chi_{lt} = \begin{pmatrix} \tilde{X}'_{yz} + Y_{3a} + 5Y_{3u} + X_{4a} - X_{4v}^{\alpha} & -2Y_x + \tilde{X}'_{zx} + Y_{3b} + Y_{3v} + X_{4b} - 3X_{4u}^{\alpha} & 2Y_z + \tilde{X}'_{xy} - Y_z^{\alpha} + Y_z^{\beta} + X_{4v}^{\beta 1} - X_{4v}^{\beta 2} \\ 2Y_x + \tilde{X}'_{yz} - Y_{3a} - Y_{3u} - X_{4a} - 3X_{4v}^{\alpha} & \tilde{X}'_{zx} + Y_{3b} - 5Y_{3v} - X_{4b} - X_{4u}^{\alpha} & -2Y_z + \tilde{X}'_{xy} + Y_z^{\alpha} + Y_z^{\beta} - X_{4v}^{\beta 1} - X_{4v}^{\beta 2} \\ -2Y_x + \tilde{X}'_{yz} - 4Y_{3u} + 4X_{4v}^{\alpha} & 2Y_y + \tilde{X}'_{zx} + 4Y_{3v} + 4X_{4u}^{\alpha} & \tilde{X}'_{xy} - 2Y_z^{\beta} + 2X_{4v}^{\beta 2} \end{pmatrix}, \quad (G6)$$

$$\chi_{tl} = \begin{pmatrix} \tilde{X}'_{yz} - Y_{3a} - 5Y_{3u} + X_{4a} - X_{4v}^{\alpha} & -2Y_x + \tilde{X}'_{yz} + Y_{3a} + Y_{3u} - X_{4a} - 3X_{4v}^{\alpha} & 2Y_x + \tilde{X}'_{yz} + 4Y_{3u} + 4X_{4v}^{\alpha} \\ 2Y_y + \tilde{X}'_{zx} + Y_{3b} - Y_{3v} + X_{4b} - 3X_{4u}^{\alpha} & \tilde{X}'_{zx} - Y_{3b} + 5Y_{3v} - X_{4b} - X_{4u}^{\alpha} & -2Y_y + \tilde{X}'_{zx} - 4Y_{3v} + 4X_{4u}^{\alpha} \\ -2Y_z + \tilde{X}'_{xy} + Y_z^{\alpha} - Y_z^{\beta} + X_{4v}^{\beta 1} - X_{4v}^{\beta 2} & 2Y_z + \tilde{X}'_{xy} - Y_z^{\alpha} - Y_z^{\beta} - X_{4v}^{\beta 1} - X_{4v}^{\beta 2} & \tilde{X}'_{xy} + 2Y_z^{\beta} + 2X_{4v}^{\beta 2} \end{pmatrix}, \quad (G7)$$

$$\chi_{tt} = \begin{pmatrix} 3X_0 + 3X_u - 3X_v - 4X_{40} - X_{4u}^{\beta 2} & -Y_z + 3X_{xy} - 2Y_z^{\alpha} + 2X_{4v}^{\beta 2} & Y_y + 3X_{zx} - Y_{3b} - 3Y_{3v} - X_{4b} - X_{4u}^{\alpha} \\ Y_z + 3X_{xy} + 2Y_z^{\alpha} + 2X_{4v}^{\beta 2} & 3X_0 + 3X_u + 3X_v - 4X_{40} + X_{4u}^{\beta 2} & -Y_x + 3X_{yz} - Y_{3a} + 3Y_{3u} + X_{4a} - X_{4v}^{\alpha} \\ -Y_y + 3X_{zx} + Y_{3b} + 3Y_{3v} - X_{4b} - X_{4u}^{\alpha} & Y_x + 3X_{yz} + Y_{3a} - 3Y_{3u} + X_{4a} - X_{4v}^{\alpha} & 3X_0 - 6X_u + X_{40} - X_{4u}^{\beta 1} \end{pmatrix}, \quad (G8)$$

where the following relations with respect to the octupoles and hecadcapoles are used as

$$\begin{aligned} Y_{3a} &= \frac{1}{4}(5Y_x^{\alpha} - 3Y_x^{\beta}), \quad Y_{3b} = -\frac{1}{4}(5Y_y^{\alpha} + 3Y_y^{\beta}), \quad Y_{3u} = -\frac{1}{4}(Y_x^{\alpha} + Y_x^{\beta}), \quad Y_{3v} = -\frac{1}{4}(Y_y^{\alpha} - Y_y^{\beta}), \\ X_{40} &= \frac{1}{4}(X_4 + X_{4u}), \quad X_{4u}^{\alpha} = \frac{1}{4}(X_{4y}^{\alpha} - X_{4y}^{\beta}), \quad X_{4v}^{\alpha} = -\frac{1}{4}(X_{4x}^{\alpha} + X_{4x}^{\beta}), \quad X_{4u}^{\beta 1} = \frac{1}{4}(5X_4 - 7X_{4u}), \quad X_{4v}^{\beta 1} = X_{4z}^{\alpha}, \\ X_{4u}^{\beta 2} &= -X_{4v}, \quad X_{4v}^{\beta 2} = X_{4z}^{\beta}, \quad X_{4a} = -\frac{1}{4}(X_{4x}^{\alpha} - 7X_{4x}^{\beta}), \quad X_{4b} = -\frac{1}{4}(X_{4y}^{\alpha} + 7X_{4y}^{\beta}), \end{aligned} \quad (G9)$$

in $\chi^{[0 \times 3]}$, $\chi^{[1 \times 3]}$ and $\chi^{[2 \times 2]}$, while

$$X_{3a} = \frac{1}{2}(5X_x^{\alpha} - 3X_x^{\beta}), \quad X_{3b} = -\frac{1}{2}(5X_y^{\alpha} + 3X_y^{\beta}), \quad X_{3u} = -\frac{1}{2}(X_x^{\alpha} + X_x^{\beta}), \quad X_{3v} = -\frac{1}{2}(X_y^{\alpha} - X_y^{\beta}) \quad (G10)$$

in $\chi^{[1 \times 2]}$.

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