



Axial point groups: rank 1, 2, 3 and 4 property tensor tables

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The form of a physical property tensor of a quasi-one-dimensional material such as a nanotube or a polymer is determined from the material's axial point group. Tables of the form of rank 1, 2, 3 and 4 property tensors are presented for a wide variety of magnetic and non-magnetic tensor types invariant under each point group in all 31 infinite series of axial point groups. An application of these tables is given in the prediction of the net polarization and magnetic-field-induced polarization in a one-dimensional longitudinal conical magnetic structure in multiferroic hexaferrites.

1. Introduction

A considerable amount of literature exists on the derivation and tabulation of the form of physical property tensors invariant under non-magnetic crystallographic point groups (Jahn, 1949; Nye, 1957; Wooster, 1973; Kopský, 1979*a*; Sirotin & Shaskolskaya, 1982; Brandmüller & Winter, 1985; Litvin & Litvin, 1990; and references contained in these sources) and under magnetic crystallographic point groups (Sirotin, 1962; Birss, 1964; Tenenbaum, 1966; Kopský, 1976, 1979*b*; Litvin & Litvin, 1991; Authier, 2003; and references contained in these sources). The symmetry of quasi-one-dimensional materials, such as polymers (Vainshtein, 1966) and nanotubes (Damnjanović & Milošević, 2010), is described by non-magnetic and magnetic *line groups* (Hermann, 1928; Alexander, 1929; Damnjanović & Vujičić, 1982). The point groups of these line groups, called *axial point groups*, are the invariance groups of the physical properties of such one-dimensional materials and determine the form of the tensors representing their physical properties.

The 31 families of non-magnetic and magnetic axial point-group types (Damnjanović & Vujičić, 1981) are listed in Table 1. Each family consists of an infinite number of point groups. These families of axial point groups are subdivided into three subclasses: (i) families of groups \mathbf{G} which do not contain the time inversion operation $1'$, neither by itself nor coupled with another element; (ii) families of groups $\mathbf{G}1'$ which are direct products of a group \mathbf{G} of the first subclass and the group $1' = \{1, 1'\}$; and (iii) families of groups $\mathbf{G}(\mathbf{H}) = \mathbf{H} + (\mathbf{G} - \mathbf{H})1'$ where \mathbf{H} is a subgroup of index two of a group \mathbf{G} of the first subclass whose elements are not coupled with time inversion, and the remaining elements of \mathbf{G} , *i.e.* the elements in $\mathbf{G} - \mathbf{H}$, are coupled with the time inversion.

2. Rank 1, 2, 3 and 4 property tensor tables

We have tabulated the form of 60 rank 1, 2, 3 and 4 property tensor types invariant under each axial point group (the

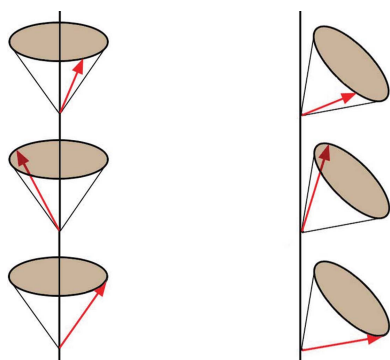


Table 1
Families of axial point-group types.

A symbol for each axial point-group family is given in the left-hand column. C_n denotes the family of axial group types with $n = 1, 2, 3, \dots$ of groups generated by a rotation of $2\pi/n$ about an axis which we take as the z axis. σ_v is a vertical mirror plane, a plane containing the z axis, σ_h a horizontal mirror plane, perpendicular to the z axis, U a twofold rotation perpendicular to the z axis, and U_d a twofold rotation perpendicular to the z axis and halfway between neighboring vertical mirror planes. In the right-hand column is the limiting group of each family of axial point groups.

Families of groups G :	Limiting group
C_n	C_∞
$C_{nv} = C_n + \sigma_v C_n$	$C_{\infty v} = C_\infty + \sigma_v C_\infty$
$S_{2n} = C_n + (\sigma_h C_{2n})' C_n$	$C_{\infty h} = C_\infty + \sigma_h C_\infty$
$C_{nh} = C_n + \sigma_h C_n$	$C_{\infty h} = C_\infty + \sigma_h C_\infty$
$D_n = C_n + U C_n$	$D_\infty = C_\infty + U C_\infty$
$D_{nd} = C_{nv} + U_d C_{nv}$	$D_{\infty h} = C_{\infty v} + \sigma_h C_{\infty v}$
$D_{nh} = C_{nv} + \sigma_h C_{nv}$	$D_{\infty h} = C_{\infty v} + \sigma_h C_{\infty v}$
Families of groups G1':	
$C_n 1' = C_n + 1' C_n$	$C_\infty 1' = C_\infty + 1' C_\infty$
$C_{nv} 1' = C_{nv} + 1' C_{nv}$	$C_{\infty v} 1' = C_{\infty v} + 1' C_{\infty v}$
$S_{2n} 1' = S_{2n} + 1' S_{2n}$	$C_{\infty h} 1' = C_{\infty h} + 1' C_{\infty h}$
$C_{nh} 1' = C_{nh} + 1' C_{nh}$	$C_{\infty h} 1' = C_{\infty h} + 1' C_{\infty h}$
$D_n 1' = D_n + 1' D_n$	$D_\infty 1' = D_\infty + 1' D_\infty$
$D_{nd} 1' = D_{nd} + 1' D_{nd}$	$D_{\infty h} 1' = D_{\infty h} + 1' D_{\infty h}$
$D_{nh} 1' = D_{nh} + 1' D_{nh}$	$D_{\infty h} 1' = D_{\infty h} + 1' D_{\infty h}$
Families of groups G(H):	
$C_{2n}(C_n) = C_n + C_{2n}' C_n$	$C_\infty 1' = C_\infty + 1' C_\infty$
$S_{2n}(C_n) = C_n + (\sigma_h C_{2n})' C_n$	$C_{\infty h}(C_\infty) = C_\infty + \sigma_h' C_\infty$
$C_{nh}(C_n) = C_n + \sigma_h' C_n$	$C_{\infty h}(C_\infty) = C_\infty + \sigma_h' C_\infty$
$C_{2nh}(S_{2n}) = S_{2n} + \sigma_h' S_{2n}$	$C_{\infty h} 1' = C_{\infty h} + 1' C_{\infty h}$
$C_{2nh}(C_{nh}) = C_{nh} + C_{2n}' C_{nh}$	$C_{\infty h} 1' = C_{\infty h} + 1' C_{\infty h}$
$D_n(C_n) = C_n + U' C_n$	$D_\infty(C_\infty) = C_\infty + U' C_\infty$
$D_{2n}(D_n) = D_n + C_{2n}' D_n$	$D_\infty 1' = D_\infty + 1' D_\infty$
$C_{nv}(C_n) = C_n + \sigma_v' C_n$	$C_{\infty v}(C_\infty) = C_\infty + \sigma_v' C_\infty$
$C_{2nv}(C_{nv}) = C_{nv} + C_{2n}' C_{nv}$	$C_\infty 1' = C_\infty + 1' C_\infty$
$D_{nd}(S_{2n}) = S_{2n} + U_d' S_{2n}$	$D_{\infty h}(C_{\infty h}) = C_{\infty h} + \sigma_v' C_{\infty h}$
$D_{nd}(D_n) = D_n + \sigma_v' D_n$	$D_{\infty h}(D_\infty) = D_\infty + \sigma_h' D_\infty$
$D_{nd}(C_{nv}) = C_{nv} + U_d' C_{nv}$	$D_{\infty h}(C_{\infty v}) = C_{\infty v} + \sigma_h' C_{\infty v}$
$D_{nh}(C_{nh}) = C_{nh} + \sigma_v' C_{nh}$	$D_{\infty h}(C_{\infty h}) = C_{\infty h} + \sigma_v' C_{\infty h}$
$D_{nh}(D_n) = D_n + \sigma_h' D_n$	$D_{\infty h}(D_\infty) = D_\infty + \sigma_h' D_\infty$
$D_{nh}(C_{nv}) = C_{nv} + \sigma_h' C_{nv}$	$D_{\infty h}(C_{\infty v}) = C_{\infty v} + \sigma_h' C_{\infty v}$
$D_{2nh}(D_{nd}) = D_{nd} + C_{2n}' D_{nd}$	$D_{\infty h} 1' = D_{\infty h} + 1' D_{\infty h}$
$D_{2nh}(D_{nh}) = D_{nh} + C_{2n}' D_{nh}$	$D_{\infty h} 1' = D_{\infty h} + 1' D_{\infty h}$

complete tables are available as supporting information). These property tensors are defined in terms of the four types of rank 0 property tensor types denoted by 1, e , a and ae . These rank 0 tensors are defined in Table 2 by their transformation properties under the action of spatial inversion $\bar{1}$ and time inversion $1'$. The rank 0 tensor given in the i th row of the left-hand-side column transformed by the element in the j th column of the top row is given at the intersection of the i th row and j th column.

We list the 60 rank 1, 2, 3 and 4 property tensor types which we consider in Table 3. These tensors are given in terms of a rank 0 tensor and products of the polar vector tensor V . The symbols [] and { }, as in $[V^2]$ and $\{V^2\}$, denote the symmetrization and anti-symmetrization, respectively, of the tensors contained within the symbol. The Birss (1964) nomenclature of the type of each tensor is given in the top row of each column of tensors: tensors of rank n are called *polar* if they transform under rotations and rotation-inversions as a product of n vectors; and *axial* if an additional sign change

Table 2
Transformation properties of rank 0 property tensors under spatial inversion $\bar{1}$ and time inversion $1'$.

Transformation	1	$\bar{1}$	$1'$	$\bar{1}'$
Rank 0	1	1	1	1
Property tensor	e	e	$-e$	e
	a	a	a	$-a$
	ae	ae	$-ae$	$-ae$

Table 3
Tensor types of rank 1, 2, 3 and 4.

These tensors are denoted using Jahn notation (Jahn, 1949). ' V ' represents a three-dimensional polar vector and $V^m = V \times V \times \dots \times V$ the m th ranked product of V . ' e ' and ' a ' are zero-rank tensors that change sign under spatial inversion $\bar{1}$ and time inversion $1'$, respectively.

	i polar	i axial	c polar	c axial
Rank 1	V	eV	aV	aeV
Rank 2	V^2 [V^2] { V^2 }	eV^2 $e[V^2]$ $e\{V^2\}$	aV^2 $a[V^2]$ $a\{V^2\}$	aeV^2 $ae[V^2]$ $ae\{V^2\}$
Rank 3	V^3 [V^3] $V[V^2]$ { V^2 } V	eV^3 $e[V^3]$ $eV[V^2]$ $e\{V^2\}V$	aV^3 $a[V^3]$ $aV[V^2]$ $a[V^2]V$	aeV^3 $ae[V^3]$ $aeV[V^2]$ $ae[V^2]V$
Rank 4	V^4 [V^4] $V[V^3]$ [[V^2] 2] [V^2] 2 [(V^2) 2] [V^2] V^2	eV^4 $e[V^4]$ $eV[V^3]$ $e[[V^2]^2]$ $e[V^2]^2$ $e[(V^2)^2]$ $e[V^2]V^2$	aV^4 $a[V^4]$ $aV[V^3]$ $a[[V^2]^2]$ $a[V^2]^2$ $a[(V^2)^2]$ $a[V^2]V^2$	aeV^4 $ae[V^4]$ $aeV[V^3]$ $ae[[V^2]^2]$ $ae[V^2]^2$ $ae[(V^2)^2]$ $ae[V^2]V^2$

occurs for rotation-inversions. i and c tensors are, respectively, invariant or change sign under time inversion $1'$.

The derivation of the form of a property tensor invariant under a non-magnetic group first uses the fact that since non-magnetic groups do not contain the time inversion operation, the forms of a c polar tensor and a c axial tensor are, respectively, identical with their corresponding i polar tensor and i axial tensor. That is, for example, the forms of the property tensors aV^2 and aeV^2 , invariant under any non-magnetic group, are identical, respectively, with the forms of the property tensors V^2 and eV^2 invariant under the same non-magnetic group. The form of i polar and i axial tensors invariant under non-magnetic groups can almost always be either directly found in the tables of Sirotni & Shaskolskaya (1982), or by a coordinate transformation of a form found in these tables (see the example below). There are cases when the non-magnetic group is not one considered in these tables, such as $\bar{8}m2$. The form of tensors invariant under such point groups is derived using Neumann's principle (Birss, 1964).

The derivation of the form of a property tensor invariant under a magnetic group is done using the methodology of Litvin (1994). It is shown there that the form of any property tensor invariant under a magnetic group is the same as the form of an i polar or i axial property tensor invariant under a related non-magnetic group. For a given property tensor and

Table 4
Piezomagnetic tensors invariant under the axial point groups of the axial point-group family $\mathbf{D}_{2n}(\mathbf{D}_n)$.

$n = 1$	$\mathbf{D}_2(\mathbf{D}_1) = 2_x 2_y 2_z (2_y) = 2_x' 2_y 2_z'$	$\begin{pmatrix} 0 & 0 & 0 & 0 & 0 & xxy \\ yxx & yyy & yzz & 0 & 0 & 0 \\ 0 & 0 & 0 & zyz & 0 & 0 \end{pmatrix}$	
$n = 2$	$\mathbf{D}_4(\mathbf{D}_2) = 4_z 2_x 2_{xy} (2_x 2_y 2_z) = 4_z' 2_x 2_{xy}'$	$\begin{pmatrix} 0 & 0 & 0 & xyz & 0 & 0 \\ 0 & 0 & 0 & 0 & xyz & 0 \\ 0 & 0 & 0 & 0 & 0 & zxy \end{pmatrix}$	
$n = 3$	$\mathbf{D}_6(\mathbf{D}_3) = 6_z 2_x 2_1 (3_z 2_x) = 6_z' 2_x 2_1'$	$\begin{pmatrix} xxx & -xxx & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & -xxx \\ 0 & 0 & 0 & 0 & 0 & 0 \end{pmatrix}$	$\begin{pmatrix} xxx & xyy & xzz & xyz & xxz & xxy \\ yxx & yyy & yzz & yyz & yxz & yxy \\ zxx & zyy & zzz & zyz & zxz & zxy \end{pmatrix}$
$n = \infty$	$\mathbf{D}_{\infty} 1' = \infty 21'$	$\begin{pmatrix} 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 \end{pmatrix}$	

magnetic group, the corresponding i polar or i axial property tensor and related non-magnetic group are found, see the example below, and then its form is determined as above.¹

While each family of axial point groups contains an infinite number of groups, for a specific tensor of rank m , one does not have to tabulate the form of the tensor for each of the infinity of groups in the family. This follows from the following theorem (Hermann, 1934; Litvin, 2014):

The form of an m th rank physical property tensor invariant under an axial point group which contains the subgroup C_n , with $n > m$, is invariant under the limiting group of that axial point-group family.

The limiting group of each axial point-group family, the axial point group of that family as n goes to infinity, is given in Table 1. Consequently, if one is to determine the form of an m th rank tensor invariant under all axial point groups of a specific family, one needs only to determine the form of the tensor for those axial point groups with $n = 1, 2, \dots, m$ and $n = \infty$. The form of the tensor for all $n > m$ is the same as for $n = \infty$.

¹ The tables presented in this paper were not computer generated. They were systematically checked and compared to existing tabulations: rank 2 and 3 property tensors of axial point groups which are non-magnetic and magnetic crystallographic point groups were compared with and agree with the results of Litvin & Litvin (1991). Rank 2 property tensors of axial point groups which are non-magnetic crystallographic point groups were also compared with and agree with the results of Damnjanović *et al.* (1999). In Table 5.5 of Damnjanović & Milošević (2010) we find that their $n = 2$ case of the groups C_{2n} , the point group $2_x m_x m_y$, the symmetric polar (in Birss nomenclature) second-rank tensor $[V^2]$ does not agree with these tables nor with those of Sirotin & Shaskolskaya (1982).

For example, consider the form of the piezomagnetic tensor, a tensor of the type $aeV[V^2]$, invariant under the magnetic axial point groups of the axial point-group family $\mathbf{D}_{2n}(\mathbf{D}_n)$. Since this is a tensor of rank $m = 3$, one needs only to tabulate the form of this tensor for the axial point groups with $n = 1, 2, 3$ and ∞ . These piezomagnetic tensors are given in Table 4. Since this tensor is symmetric in the last two indices, *i.e.* $aeV[V^2]_{JKL} = aeV[V^2]_{JLK}$, in tabulating this tensor we use the following abbreviated tensor format (Sirotin & Shaskolskaya, 1982):

For $n = 1$: the form of the property tensor $aeV[V^2]$ invariant under $\mathbf{D}_2(\mathbf{D}_1) = 2_x 2_y 2_z (2_y) = 2_x' 2_y 2_z'$ is the same as the property tensor $V[V^2]$ invariant under $\mathbf{m}_x \mathbf{m}_z 2_y$ (Litvin, 1994). The form of this property tensor invariant under $\mathbf{m}_x \mathbf{m}_y 2_z$ is found in Sirotin & Shaskolskaya (1982) and a coordinate transformation gives the form under $\mathbf{m}_x \mathbf{m}_z 2_y$ (see Table 4).

For $n = 2$ and 3: the forms of the property tensor $aeV[V^2]$ invariant under $\mathbf{D}_4(\mathbf{D}_2) = 4_z 2_x 2_{xy} (2_x 2_y 2_z) = 4_z' 2_x 2_{xy}'$ and $\mathbf{D}_6(\mathbf{D}_3) = 6_z 2_x 2_1 (3_z 2_x) = 6_z' 2_x 2_1'$ are the same as the property tensor $V[V^2]$ invariant under, respectively, $4_z 2_x \mathbf{m}_{xy}$ and $6_z 2_x \mathbf{m}_1$, the forms of which can be found in Sirotin & Shaskolskaya (1982) (see Table 4).

For $n = \infty$: the form of the property tensor $aeV[V^2]$ invariant under $\mathbf{D}_{\infty} 1' = \infty 21'$ is the null tensor since $aeV[V^2]$ is a c tensor and the magnetic group contains the element $1'$ (see Table 4).

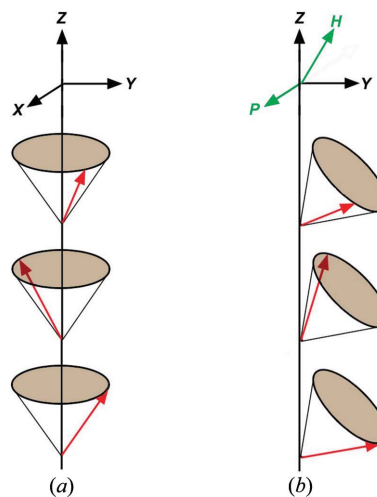
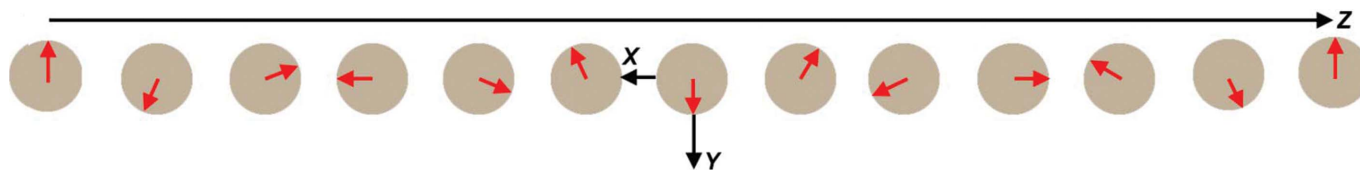


Figure 1
(a) The longitudinal conical magnetic structure in Sc-substituted barium hexaferrite; the pitch of the helix is 150° and the half cone angle 30°. (b) A polarization P can be induced by applying a magnetic field H in the Y - Z plane.


Figure 2

The longitudinal conical magnetic structure showing each cone as it would be viewed looking down the z axis in Fig. 1(a). The orientation of the spin of each cone is related to the orientation of its neighbor by a rotation of 150° about the z axis. The twofold rotation around the x axis at the origin shown coupled with time inversion is a symmetry of the magnetic structure.

3. Magnetoelectric effect in multiferroic hexaferrites

The longitudinal conical magnetic structure in Sc-substituted barium hexaferrite $\text{BaFe}_{12-x}\text{Sc}_x\text{O}_{19}$, with $x = 1.8$ (Aleshko-Ozhevskii *et al.*, 1968, 1969), is shown in Fig. 1(a). The pitch of the helix is 150° and the half cone angle 30° . According to the inverse Dzyaloshinskii–Moriya model, the structure in Fig. 1(a) has no net polarization, but a polarization can be induced by tilting the cone axis with the use of a magnetic field (Tokunaga *et al.*, 2010). This is shown in Fig. 1(b) where a magnetic field in the Y – Z plane induces, as predicted by the inverse Dzyaloshinskii–Moriya model, a polarization in the X direction. These results, no net polarization in Fig. 1(a) and the magnetic-field-induced polarization in the X direction, can be predicted by considering the axial point-group symmetry of the longitudinal conical magnetic structure in Fig. 1(a) and the form of the polarization and magnetoelectric effect tensors invariant under this point group.

The magnetic structure in Fig. 1(a) is invariant under the translational symmetry element ($R_{5/12}^Z | 001$), where $R_{5/12}^Z$ is a rotation of 150° about the z axis. In addition (see Fig. 2), the point group of this magnetic structure contains a symmetry $2'$, a twofold rotation perpendicular to the z axis coupled with time inversion. Consequently, the axial point group of this structure is $\mathbf{C}_{12} + 2'\mathbf{C}_{12} = \mathbf{D}_{12}(\mathbf{C}_{12})$. With the axial point group $\mathbf{D}_{12}(\mathbf{C}_{12})$, a point group $\mathbf{D}_n(\mathbf{C}_n)$ with $n = 12$, polarization, a rank $m = 1$ tensor of the type eV , and the magnetoelectric tensor, of rank $m = 2$ tensor of the type aeV^2 , we have for both property tensors $n > m$. Consequently, the form of the polarization and magnetoelectric tensors invariant under $\mathbf{D}_{12}(\mathbf{C}_{12})$ is that of the tensors invariant under $\mathbf{D}_\infty(\mathbf{C}_\infty)$. From the axial point-group property tables we find for the point group $\mathbf{D}_\infty(\mathbf{C}_\infty)$ that a tensor of the type eV vanishes and therefore there is no net polarization in the longitudinal conical magnetic structure in Fig. 1(a). We also have that a tensor of the type aeV^2 , the magnetoelectric tensor, is

$$\begin{pmatrix} 0 & \alpha_{xy} & 0 \\ -\alpha_{xy} & 0 & 0 \\ 0 & 0 & 0 \end{pmatrix}.$$

Consequently, for a magnetic field in the Y – Z plane one would then predict a polarization in the X direction given by $P_x = \alpha_{xy}H_y$.

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