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A Simplified Calculation and Tabulation of Tensorial Covariants for Magnetic Point Groups Belonging to the Same Laue Class

BY VOJTĚCH KOPSKÝ

Institute of Physics, Czechoslovak Academy of Sciences, Na Slovance 2, *POB* 24, 180 40 *Praha* 8, *Czechoslovakia*

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Abstract

Four types of static tensors can be distinguished according to their parity with respect to space inversion and to time reversal. However, all magnetic point groups belonging to the same (oriented) Laue class consist, apart from inversions, of the same proper rotations. Tensors differing only by parities transform identically under the same proper rotations; their transformation properties under different groups of the same Laue class may therefore differ only by an additional change of sign, which depends on the tensor parity and on the way in which inversions are combined with proper rotations in a given group. It is shown that, for a certain natural choice of typical representations of magnetic point groups of the same Laue class, it is sufficient to calculate tensorial covariants (symmetry-adapted tensorial bases) of even parity with respect to both space inversion and time reversal for the group of proper rotations. Tensorial covariants of other parities and for other magnetic point groups of the same Laue class can then be obtained by the use of a simple conversion table and of parity arguments. The scheme is illustrated by an example from the Laue class D_4.

1. Introduction

In the preceding paper (Kopský, 1979) it has been shown how to find tensorial covariants with the help of standard tables of Clebsch–Gordan products (Kopský, 1976*a*, *b*). Lists of tensorial covariants were also given for the 32 crystal point groups and for tensors up to the fourth rank describing nonmagnetic properties.

It is desirable, especially for the purposes of the phenomenological phase transition theory, to know

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tensorial covariants for the 122 magnetic point groups and for tensors of properties connected with the application of the external magnetic field. We can, of course, perform the routine calculations in the same way as before for each of the groups. The volume of the work and of the tables will, however, substantially increase.

The consideration of tensorial covariants can be simplified to a great extent if we take the structure of magnetic point groups and the relation between transformation properties of various tensors into account. The relationship between the equilibrium form of tensors in correlation with the symmetry groups has already been studied (Sirotin, 1962; Freeman & Schmid, 1975; Kopský, 1976*c*). The theory of tensorial covariants gives even better insight into the situation than do these studies; while the equilibrium tensors are unambiguously determined by the symmetry group, the tensorial covariants also still depend on the choice of REP's (irreducible or physically irreducible representations) with which we associate them. It appears that the most natural choice of typical representations also leads to the clearest relationship between covariants for different groups belonging to the same Laue classes. This paper describes the choice of REP's, elucidates the relation between covariants, and demonstrates the simple scheme which arises by an example from the Laue class D_4.

In the following we use the Schoenflies notation for magnetic classes (Dimmock & Wheeler, 1966) and the international notation (Opechowski & Guccione, 1965) with indices specifying the orientation of generators for specifically oriented groups. Space inversion is denoted by i, time reversal by e', and their combination by i'. Special symbols are used for the three inversion groups: $I = C_i - \bar{1} = \{e,i\}$; $E' = C_1' = 1' = \{e,e'\}$; $I' = C_i(C_1) = \bar{1}' = \{e,i'\}$; and for the full inversion group $E_0 = C_i' = \bar{1}1' = \{e,i,e',i'\}$. The symbols $\mathrm{SO}(3)$, $\mathrm{O}(3) = \mathrm{SO}(3) \times I$, and $\mathrm{O}'(3) = \mathrm{O}(3) \times E' = \mathrm{SO}(3) \times E_0$ mean the proper orthogonal group, the full orthogonal group, and the general space–time rotation group [the last term is taken from Opechowski (1974) (this paper is also included in Freeman & Schmid, 1975)], which contains all magnetic point groups (including noncrystallographic ones).

2. The four kinds of tensors

In classical physics we distinguish four types of tensors according to their parities with respect to space inversion i and to time reversal e'. The simplest tensors are the four scalars: the trivial or i-scalar, the i-pseudoscalar ε, the c-scalar τ, and the c-pseudoscalar $\varepsilon\tau$. Each of the scalars is invariant under the proper rotation group $\mathrm{SO}(3)$ and belongs to one of the four REP's Γ_μ^ν of the full inversion group E_0, where $\nu = +, -$, and $\mu = e, m$, denote the even and odd parities with respect to i and e' respectively. With reference to the group $\mathrm{O}'(3)$ the scalars transform according to the four possible scalar REP's $\mathrm{D}_\mu^{(0)\nu} = \mathrm{D}^{(0)}.\ \Gamma_\mu^\nu$, where $\mathrm{D}^{(0)}$ is the scalar (identity) REP of $\mathrm{SO}(3)$.

There are also four types of vectors: pseudovectors $\mathbf{p} = x_{pi}\mathbf{e}_i$, ordinary vectors $\mathbf{v} = x_{vi}\mathbf{e}_i$, magnetic-type vectors $\mathbf{m} = x_{mi}\mathbf{e}_i$, and current* (velocity)-type vectors $\mathbf{j} = x_{ji}\mathbf{e}_i$. Each of these four vectors forms a carrier space $\mathrm{L}_{3\mu}^\nu$ for one of the four vector REP's V_μ^ν of the group $\mathrm{O}'(3)$. Each of these REP's assigns to the element $g \in \mathrm{O}'(3)$ an operator $\mathrm{V}_\mu^\nu(g)$ or, using letters instead of parity labels, $\mathrm{P}(g)$, $\mathrm{V}(g)$, $\mathrm{M}(g)$, and $\mathrm{J}(g)$, which acts on the space L_{3e}^+, L_{3e}^-, L_{3m}^+, and L_{3m}^- respectively. In appropriate complex bases, these are the four vector REP's $\mathrm{D}_\mu^{(1)\nu} = \mathrm{D}^{(1)}.\ \Gamma_\mu^\nu$ of the group $\mathrm{O}'(3)$, derived from the vector REP $\mathrm{D}^{(1)}$ of $\mathrm{SO}(3)$, known from the theory of quantum angular momenta (Lyubarskii, 1958). In Table 1 we give the REP's Γ_μ^ν, the symbols for scalar and vector quantities, and the names of scalars and vectors according to Birss (1962, 1963, 1964) (these are used here).

A general tensor of rank $k = k_e^+ + k_e^- + k_m^+ + k_m^-$ is an element of direct product of direct powers of spaces $\mathrm{L}_{3\mu}^\nu$ and we have to distinguish its partial ranks k_e^+, k_e^-, k_m^+, and k_m^- in pseudovector, vector, magnetic-vector, and current-vector indices respectively. The space of such tensors carries a representation A of the group $\mathrm{O}'(3)$ which assigns to each element $g \in \mathrm{O}'(3)$ an operator

$$\mathrm{A}(g) = \mathrm{P}^{k_e^+}(g) \otimes \mathrm{V}^{k_e^-}(g) \otimes \mathrm{M}^{k_m^+}(g) \otimes \mathrm{J}^{k_m^-}(g). \qquad (1)$$

Concerning the transformation properties, which are our sole interest here, we can interpret a certain vector of the four kinds as a pseudovector multiplied by a corresponding scalar and the representation V_μ^ν as the representation P multiplied by Γ_μ^ν. Then we can rewrite (1) as

$$\mathrm{A}(g) = \Gamma_\mu^\nu . \mathrm{P}^k(g), \qquad (2)$$

where

$$\Gamma_\mu^\nu = (\Gamma_e^-)^{k_e^- + k_m^-} . (\Gamma_m^+)^{k_m^+ + k_m^-}. \qquad (3)$$

We shall, as in the preceding paper, work with adjoint spaces. Then we can write for the transformation properties of components of a tensor $\mathbf{u}$ with partial ranks k_e^+, k_e^-, k_m^+, and k_m^-:

$$\begin{aligned} & u_{i_1 i_2 \ldots i_{k_e^+},\, j_1 j_2 \ldots j_{k_e^-},\, h_1 h_2 \ldots h_{k_m^+},\, l_1 l_2 \ldots l_{k_m^-}} \\ & \sim x_{pi_1} x_{pi_2} \ldots x_{pi_{k_e^+}} . x_{vj_1} x_{vj_2} \ldots x_{vj_{k_e^-}} . \\ & \quad . x_{mh_1} x_{mh_2} \ldots x_{mh_{k_m^+}} . x_{jl_1} x_{jl_2} \ldots x_{jl_{k_m^-}} \\ & \sim (\varepsilon)^{k_e^- + k_m^-} (\tau)^{k_m^+ + k_m^-} . x_{pi_1} x_{pi_2} \ldots x_{pi_{k_e^+}} . x_{pj_1} x_{pj_2} \ldots x_{pj_{k_e^-}} . \\ & \quad . x_{ph_1} x_{ph_2} \ldots x_{ph_{k_m^+}} . x_{pl_1} x_{pl_2} \ldots x_{pl_{k_m^-}}, \end{aligned} \qquad (4)$$

* We mean here a time-reversible current which is not accompanied by entropy production. It can be physically interpreted as the superconducting current. Tensors in which the current vector indices are present appear naturally in our algebraic scheme but we have to consider them as hypothetical since their physical meaning is not yet quite clear (Ascher, 1966).

Table 1. *Irreducible representations of the full inversion group E_0 and vector representations of the general space–time rotation group* $O'(3) = SO(3) \times E_0$

REP	e	i	e'	i'	Scalar quantity	Name of (Birss) scalar	Vector REP of $O'(3)$	Name of vector	Birss name of vector
Γ_e^+	1	1	1	1	1	*i*-scalar	$\mathbf{P}$ $[D_e^{(1)+}]$	pseudovector	*i*-pseudovector
Γ_e^-	1	−1	1	−1	ε	*i*-pseudoscalar	$\mathbf{V}$ $[D_e^{(1)-}]$	vector (polar)	*i*-vector
Γ_m^+	1	1	−1	−1	τ	*c*-scalar	$\mathbf{M}$ $[D_m^{(1)+}]$	magnetic vector	*c*-pseudovector
Γ_m^-	1	−1	−1	1	$\varepsilon\tau$	*c*-pseudoscalar	$\mathbf{J}$ $[D_m^{(1)-}]$	current vector	*c*-vector

where the symbol ~ means 'transforms like'. The symmetrization or, as it is often called, the particularization of tensor indices can be performed only within those vector indices which belong to the same kind of vector. With this in mind, we can rewrite (4) in a simpler form

$$u_i \sim (\varepsilon)^{k_e^- + k_m^-}(\tau)^{k_m^+ + k_m^-}.v_i, \qquad (5)$$

where, to avoid unnecessary crowding of indices, we collect them into one index i, which comprises many vector indices and the symmetrization. Generally, many tensors $\mathbf{u}$ on the left-hand sides of relations (4) and (5) may correspond to the expressions on the right-hand sides. Corresponding tensor spaces are, of course, different but they are transformed in the same way by all elements of the group $O'(3)$ (and also by the respective group of permutation of indices).

Relations (4) or (5) separate the transformation properties of tensor $\mathbf{u}$ with respect to proper rotation group $SO(3)$ from its parities (transformation properties with respect to the full inversion group E_0). The first ones are wholly contained in the tensor $\mathbf{v}$, while the parities are defined by the product $(\varepsilon)^{k_e^- + k_m^-}(\tau)^{k_m^+ + k_m^-}$, which is one of the four scalars. We shall say that $\mathbf{u}$ is a 1_μ^ν tensor if the parities belong to the REP Γ_μ^ν of E_0. Evidently, any tensor belongs to one of the four 1_μ^ν types. Correlation of this parity nomenclature with the usual nomenclature (where the adjective 'axial' and the prefix 'pseudo' are used on the same basis) and with a terminology used in the Russian literature is given in Table 2.

Table 2. *Correlation of tensor classifications*

This paper *k*th rank	Birss *k* even	Birss *k* odd	Russian literature
1_e^+-tensor	polar *i*-tensor	axial *i*-tensor	even-type tensor
1_e^--tensor	axial *i*-tensor	polar *i*-tensor	electric-type tensor
1_m^+-tensor	polar *c*-tensor	axial *c*-tensor	magnetic-type tensor
1_m^--tensor	axial *c*-tensor	polar *c*-tensor	electromagnetic tensor

3. Magnetic point groups belonging to the same Laue class

Let G be a proper rotation group oriented in a certain way with respect to the standard Cartesian frame of reference. We say that a magnetic point group H belongs to (oriented) Laue class G if, apart from combinations with inversions i, e', i', the group H consists of the same rotations as G. The procedure of constructing the classical groups from groups of proper rotations (Altmann, 1963) and of magnetic point groups from the classical ones [Shubnikov, 1951 (see also Shubnikov & Belov, 1964); Tavger & Zaitsev, 1956; Opechowski & Guccione, 1965; Kopský, 1976*c*] by the use of halving groups is well known and has been discussed many times. Let us recall that magnetic point groups derived in this way from a certain classical group F are said to form a magnetic family F (Opechowski & Guccione, 1965). We shall use here the fact that each halving subgroup of a given group is a kernel of an alternating REP, *i.e.* of the REP which has characters +1 or −1 only; the halving subgroup then corresponds to those elements which have characters +1. The magnetic point groups belonging to the Laue class of the group G can be classified as follows.

(i) Groups isomorphous with G – the proper rotation group. If $\Gamma_\alpha(G)$ is an alternating REP of G, then $F_\alpha = \mathrm{Ker}\,\Gamma_\alpha(G) \lhd G$ is a halving group of G. We can construct a noncentrosymmetric group $H_\alpha = F_\alpha + i(G - F_\alpha)$ by combining elements of the coset $G - F_\alpha$ with space inversion. In the same way we can construct other magnetic groups by combining the elements of the coset with e' or with i'. This will exhaust all magnetic point groups isomorphous with G, if G has only one alternating REP. If G has two such REP's $\Gamma_\alpha(G)$ and $\Gamma_\beta(G)$, then necessarily it also has a third such REP $\Gamma_\gamma(G) = \Gamma_\alpha(G).\Gamma_\beta(G)$. It is easy to show that the three corresponding halving subgroups F_α, F_β, and F_γ have a common halving subgroup (a quartering group of G) $F_{\alpha\beta\gamma} = F_\alpha \cap F_\beta \cap F_\gamma \lhd F_\alpha, F_\beta, F_\gamma$ (in fact, $F_{\alpha\beta\gamma}$ is an intersection of any two of the groups F_α, F_β, F_γ). Factorizing G with respect to $F_{\alpha\beta\gamma}$:

$$G = F_{\alpha\beta\gamma} + F_1 + F_2 + F_3, \qquad (6)$$

where $F_1 = F_\alpha - F_{\alpha\beta\gamma}$, $F_2 = F_\beta - F_{\alpha\beta\gamma}$, $F_3 = F_\gamma - F_{\alpha\beta\gamma}$, we can see that the groups isomorphous with G must have the form:

$$H = F_{\alpha\beta\gamma} + \gamma_1 F_1 + \gamma_2 F_2 + \gamma_3 F_3, \qquad (7)$$

where $e, \gamma_1, \gamma_2, \gamma_3$ form a subgroup of E_0 (γ_i are not necessarily different). Each group (7) is unambiguously characterized by two REP's $\Gamma_\alpha(G)$ and $\Gamma_\beta(G)$

in such way that the cosets $\mathrm{G} - \mathrm{F}_\alpha$, $\mathrm{G} - \mathrm{F}_\beta$ are, in the resulting group H, combined with space inversion and time reversal respectively. It should be noted that elements of the cosets are those which, in a given REP, have the characters -1. Some of these groups thus derived may belong to the same magnetic class – this will occur if there is an automorphism of G which is equivalent to the exchange of alternating REP's (such automorphism is necessarily an outer automorphism). Magnetic groups with the same $\Gamma_\alpha(\mathrm{G})$ but different $\Gamma_\beta(\mathrm{G})$ consist, apart from combinations with e', of the same elements of O(3) and belong to the same magnetic family H_α.

(ii) Groups isomorphous with $\mathrm{G}_h = \mathrm{G} \times I$ – the centrosymmetric group. We distinguish here two kinds of groups. (1) Groups of the magnetic family G_h. These are groups which can be obtained by combining elements of a coset to a halving subgroup of G_h with e'. Again, each such halving group is a kernel of an alternating REP of G_h. (2) Paramagnetic groups. To each classical group $\mathrm{H}_\alpha = \mathrm{F}_\alpha + i(\mathrm{G} - \mathrm{F}_\alpha)$ and particularly also to the group G itself there corresponds a paramagnetic group $\mathrm{H}'_\alpha = \mathrm{H}_\alpha \times E'$, isomorphous with G_h. It can be shown that by this are exhausted all groups of the (oriented) Laue class G isomorphous with G_h.

(iii) The centrosymmetric paramagnetic group $\mathrm{G}'_h = \mathrm{G} \times E_0$ has no isomorphs within Laue class G and contains all groups of this class as its subgroups.

4. Tensorial covariants for groups of the same Laue class

Let us suppose that we have calculated covariants of tensor **v** from relations (4) or (5) for a proper rotation group G. We want to find tensorial covariants of the tensor **u** for all groups of the (oriented) Laue class G. The form of these covariants depends on the orientation of these groups which is given by the orientation of G and on the choice of their typical representations. For a given choice of the typical representation of G, the covariants of **v** can be calculated by the use of Clebsch–Gordan products. Below we show that a certain, quite natural, choice of REP's for the isomorphs of G leads to such simple relations between covariants of tensors **v** and **u** that the latter can be found almost immediately. The explanations will be illustrated by an example from Laue class D_4 in which we start from the proper rotation group oriented as given by the symbol $4_z2_x2_{xy}$.

4.1. *Groups isomorphous with* G

An example of a choice of a typical matrix representation is given in Table 3 for the group $4_z2_x2_{xy}$. Each REP assigns to each element a matrix, but it is sufficient to give only the matrices of generators. The typical variables, written with symbols of REP's transform as follows:

$$4_z x_1 = x_1,\quad 4_z x_2 = x_2,\quad 4_z x_3 = -x_3,\ 4_z x_4 = -x_4;$$
$$2_x x_1 = x_1,\quad 2_x x_2 = -x_2,\ 2_x x_3 = x_3,\quad 2_x x_4 = -x_4;$$
$$4_z(x_5, y_5) = (y_5, -x_5),\ 2_x(x_5, y_5) = (x_5, -y_5). \qquad (8)$$

For groups isomorphous with G we use the following convention: the REP's of the same numerical label assign to an element of a group H isomorphous with G the same matrix as to its proper rotation part in the group G. All groups isomorphous with the group $4_z2_x2_{xy}$ are written in the first column of Table 4. We shall obtain their typical representations according to this convention if we replace, in Table 3, the generators 4_z and 2_x by those generators of a given group which stand in the same place in the international symbol. With such a choice, the covariants of tensor **v** will have the same form for all groups isomorphous with G, because **v** is insensitive to space inversion and time reversal.

The tensor **u** differs from the tensor **v** only by a factor $(\varepsilon)^{k_e^- + k_m^-}(\tau)^{k_m^+ + k_m^-}$ which transforms as one of the

Table 3. *Typical representation of* D_4 $(4_z2_x2_{xy})$

	4_z	2_x
$\Gamma_1(x_1)$	1	1
$\Gamma_2(x_2)$	1	-1
$\Gamma_3(x_3)$	-1	1
$\Gamma_4(x_4)$	-1	-1
$R_5^{(1)}(x_5,y_5)$	$\begin{pmatrix}0 & -1\\ 1 & 1\end{pmatrix}$	$\begin{pmatrix}1 & 0\\ 0 & -1\end{pmatrix}$

Table 4. *Magnetic point groups isomorphous with* D_4 $(4_z2_x2_{xy})$*; REP's corresponding to halving subgroups and transformation properties of nontrivial scalars*

Class	Group	i	e'	ε	τ	$\varepsilon\tau$
D_4	$4_z2_x2_{xy}$	Γ_1	Γ_1	x_1	x_1	x_1
$D_4(C_4)$	$4_z2'_x2'_{xy}$	Γ_1	Γ_2	x_1	x_2	x_2
$D_4(D_2)$	$4'_z2_x2'_{xy}$	Γ_1	Γ_3	x_1	x_3	x_3
	$4'_z2'_x2_{xy}$	Γ_1	Γ_4	x_1	x_4	x_4
C_{4v}	$4_zm_xm_{xy}$	Γ_2	Γ_1	x_2	x_1	x_2
$C_{4v}(C_4)$	$4_zm'_xm'_{xy}$	Γ_2	Γ_2	x_2	x_2	x_1
$C_{4v}(C_{2v})$	$4'_zm_xm'_{xy}$	Γ_2	Γ_3	x_2	x_3	x_4
	$4'_zm'_xm_{xy}$	Γ_2	Γ_4	x_2	x_4	x_3
D_{2d}	$\bar{4}_z2_xm_{xy}$	Γ_3	Γ_1	x_3	x_1	x_3
$D_{2d}(S_4)$	$\bar{4}_z2'_xm'_{xy}$	Γ_3	Γ_2	x_3	x_2	x_4
$D_{2d}(D_2)$	$\bar{4}'_z2_xm'_{xy}$	Γ_3	Γ_3	x_3	x_3	x_1
$D_{2d}(C_{2v})$	$\bar{4}'_z2'_xm_{xy}$	Γ_3	Γ_4	x_3	x_4	x_2
D_{2d}	$\bar{4}_zm_x2_{xy}$	Γ_4	Γ_1	x_4	x_1	x_4
$D_{2d}(S_4)$	$\bar{4}_zm'_x2'_{xy}$	Γ_4	Γ_2	x_4	x_2	x_3
$D_{2d}(C_{2v})$	$\bar{4}'_zm_x2'_{xy}$	Γ_4	Γ_3	x_4	x_3	x_2
$D_{2d}(D_2)$	$\bar{4}'_zm'_x2_{xy}$	Γ_4	Γ_4	x_4	x_4	x_1

typical variables belonging to a one-dimensional (identity or alternating) REP of the group in question. If this factor is the trivial scalar, then it transforms like x_1 for all groups isomorphous with G; the covariants of tensor **u** are the same for all these groups and have the same form as the covariants of tensor **v**. Otherwise, the factor is either ε, τ or their product $\varepsilon\tau$. If, for a given group, the space inversion is combined with elements of the coset $\mathsf{G} - \mathsf{F}_\alpha$ to the subgroup $\mathsf{F}_\alpha = \operatorname{Ker} \Gamma_\alpha(\mathsf{G})$, the time reversal with elements of the coset $\mathsf{G} - \mathsf{F}_\beta$ to the subgroup $\mathsf{F}_\beta = \operatorname{Ker} \Gamma_\beta(\mathsf{G})$, then, under this group, ε transforms like x_α, τ like x_β, and $\varepsilon\tau$ like the product $x_\alpha x_\beta \sim x_\nu$. For groups isomorphous with $4_z 2_x 2_{xy}$ we give the REP's $\Gamma_\alpha(\mathsf{G})$, $\Gamma_\beta(\mathsf{G})$ in columns under i and e', the variables x_α, x_β, and x_ν in columns under ε, τ, and $\varepsilon\tau$ in Table 4.

The relationship between covariants of **v** and **u** can be found from a simple conversion table which shows how transformation properties of variables change when multiplied by a variable x_α, belonging to an alternating REP $\Gamma_\alpha(\mathsf{G})$. This conversion table is part of the Clebsch–Gordan table and we give it for the groups $4_z 2_x 2_{xy}$ as Table 5. The first row lists the typical variables for the group, the first column the variables belonging to alternating REP's. On the intersection are given the resulting typical variables.

Table 5. *Conversion table*

x_1	x_2	x_3	x_4	(x_5, y_5)
x_2	x_1	x_4	x_3	$(y_5, -x_5)$
x_3	x_4	x_1	x_2	$(x_5, -y_5)$
x_4	x_3	x_2	x_1	(y_5, x_5)

4.2. *Groups isomorphous with* G_h

Here it is suitable to choose the REP's in a different manner for groups of magnetic family G_h and for the paramagnetic isomorphs of G_h.

4.2.1. *Groups of magnetic family* G_h. The number of REP's of G_h is twice that of G and we distinguish them by parity labels + and −. If $\Gamma_\alpha(\mathsf{G})$ assigns a matrix $\mathsf{D}^{(\alpha)}(g)$ to an element $g \in \mathsf{G}$, then $\Gamma^+(\mathsf{G})$ assigns this matrix to both g and ig, while $\Gamma^-(\mathsf{G})$ assigns this matrix to g and its negative to ig. To an element $g \in \mathsf{G}_h$ there corresponds, in a given magnetic group of the family G_h, either g or $g' = e'g$. For REP's of magnetic groups we use the following convention: the REP of the same numerical and parity label assigns the same matrix to an element $g \in \mathsf{G}_h$ as to the corresponding element g or g' of a magnetic group.

Then, if a certain set of linear combinations of components of tensor **v** forms a Γ_α covariant for the group G, it evidently forms a Γ_α^+ covariant for all groups of the magnetic family G_h. The pseudoscalar transforms like x_1^- and accordingly the same set of linear combinations from components of a tensor εv forms a Γ_α^- covariant for all groups of the magnetic family G_h. To find the transformation properties of τ**v** and of $\varepsilon\tau$**v**, we have to recall that, for a given group of the family, there exists an alternating REP $\Gamma_\beta^\nu(\mathsf{G}_h)$ such that the group is obtained from G_h by combining with e' those elements of G_h which have, in the REP $\Gamma_\beta^\nu(\mathsf{G}_h)$, characters −1. Hence τ transforms, in the resulting group, as x_β^ν and $\varepsilon\tau$ as $x_1^- x_\beta^\nu$. The changes in covariants can be again found by the use of the same conversion table as before, taking additionally the multiplication of parities into account. The groups of magnetic family $4_z/m_z m_x m_{xy}$, REP's which correspond to e', and typical variables which correspond to ε, τ, and $\varepsilon\tau$ are given in Table 6(*a*).

4.2.2. *Paramagnetic groups*. These groups are of the form $\mathsf{H}' = \mathsf{H} \times E'$, where H is a classical isomorph of G. Here we choose first the REP's of H in the same manner as in §4.1, and for REP's of H′ we use an additional parity label e or m, so that the REP $\Gamma_{\alpha e}(\mathsf{H}')$ assigns the same matrix $\mathsf{D}^{(\alpha)}(g)$ to $g \in \mathsf{H}$ and to $g' = e'g$, while $\Gamma_{\alpha m}(\mathsf{H}')$ assigns this matrix to g and its negative to g'.

A set of linear combinations of components of tensor **v**, which forms a Γ_α covariant in G, then forms a $\Gamma_{\alpha e}$ covariant in all these groups; τ transforms like x_{1m} and hence the same linear combinations of τ**v** form a $\Gamma\Delta_{\alpha m}$ covariant for all these groups. If ε transforms like x_β in H, then it transforms like $x_{\beta e}$ in H′ and $\varepsilon\tau$ transforms like $x_{\beta m}$ in H′. The change of covariants can be again found from the conversion table. This information for paramagnetic noncentrosymmetric groups of the (oriented) Laue class $4_z 2_x 2_{xy}$ is collected in Table 6(*b*).

Table 6. *Nonparamagnetic, noncentrosymmetric paramagnetic and centrosymmetric paramagnetic point groups*

Class	Group	e'	ε	τ	$\varepsilon\tau$
(*a*) Nonparamagnetic point groups isomorphous with D_{4h} ($4_z/m_z m_x m_{xy}$): REP's corresponding to halving subgroups and transformation properties of nontrivial scalars					
D_{4h}	$4_z/m_z m_x m_{xy}$	Γ_1^+	x_1^-	x_1^+	x_1^-
$D_{4h}(C_{4h})$	$4_z/m_z m'_x m'_{xy}$	Γ_2^+	x_1^-	x_2^+	x_2^-
$D_{4h}(D_{2h})$	$4'_z/m_z m_x m'_{xy}$	Γ_3^+	x_1^-	x_3^+	x_3^-
	$4'_z/m_z m'_x m_{xy}$	Γ_4^+	x_1^-	x_4^+	x_4^-
$D_{4h}(D_4)$	$4_z/m'_z m'_x m'_{xy}$	Γ_1^-	x_1^1	x_1^-	x_1^+
$D_{4h}(C_{4v})$	$4_z/m'_z m_x m_{xy}$	Γ_2^-	x_1^-	x_2^-	x_2^+
$D_{4h}(D_{2d})$	$4'_z/m'_z m_x m'_{xy}$	Γ_3^-	x_1^-	x_3^-	x_3^+
	$4'_z/m'_z m'_x m_{xy}$	Γ_4^-	x_1^-	x_4^-	x_4^+
(*b*) Noncentrosymmetric paramagnetic groups					
D'_4	$4_z 2_x 2_{xy} 1'$		x_{1e}	x_{1m}	x_{1m}
C'_{4v}	$4_z m_x m_{xy} 1'$		x_{2e}	x_{1m}	x_{2m}
D'_{2d}	$\bar{4}_z 2_x m_{xy} 1'$		x_{3e}	x_{1m}	x_{3m}
	$\bar{4}_z m_x 2_{xy} 1'$		x_{4e}	x_{1m}	x_{4m}
(*c*) Centrosymmetric paramagnetic group D'_{4h} ($4_z/m_z m_x m_{xy}.1'$): transformation properties of nontrivial scalars					
D'_{4h}	$4_z/m_z m_x m_{xy}.1'$		x_{1e}^-	x_{1m}^+	x_{1m}^-

4.3. *The centrosymmetric paramagnetic group* $G'_h = G \times E_0$

To each REP $\Gamma_\alpha(G)$ there correspond four REP's $\Gamma^v_{\alpha\mu}(G'_h) = \Gamma_\alpha(G).\Gamma^v_\mu(E_0)$. Accordingly, if a certain set of linear combinations of **v** forms a Γ_α covariant in G, then it forms a $\Gamma^+_{\alpha e}$ covariant in G'_h and the same combinations of $\varepsilon\mathbf{v}$, $\tau\mathbf{v}$, and $\varepsilon\tau\mathbf{v}$ form the $\Gamma^-_{\alpha e}$, $\Gamma^+_{\alpha m}$, and $\Gamma^-_{\alpha m}$ covariants in G'_h, respectively, as indicated in Table 6(*c*).

Corollary: It is sufficient to know tensorial covariants of tensors **v** with only pseudovector indices for the proper rotation group in order to find tensorial covariants of tensors **u**, related to **v** by (4) or (5), for all magnetic point groups of the (oriented) Laue class defined by this group. Tables analogous to Tables 4, 5, and 6 are easily found. Covariants of tensors **v** up to the fourth rank can be rewritten from the lists of the preceding paper. I shall finish with an illustrative example.

5. An example

In Table 7 are given some tensorial covariants of parity 1^+_e for the group $4_z2_x2_{xy}$. Notation: p_1, p_2, p_3 are the components of the pseudovector; the u_{ik} in the usual abbreviated notation $u_1 = u_{xx}$, $u_2 = u_{yy}$, $u_3 = u_{zz}$, $u_4 = 2u_{yz}$, $u_5 = 2u_{zx}$, $u_6 = 2u_{xy}$ represent the symmetric second-rank tensor which transforms like $(1/2)(p_ip'_k + p_kp'_i)$; the antisymmetric second-rank tensor is represented by the psuedovector itself, because p_i transforms like $\varepsilon_{ijk}p_jp'_k$, where ε_{ijk} is the Levi–Civita tensor, so that p_1, p_2, p_3 transform like $(p_2p'_3 - p_3p'_2)$, $(p_3p'_1 - p_1p'_3)$, $(p_1p'_2 - p_2p'_1)$ respectively; finally, δ_{ij} means the tensor which transforms like p_iu_j ($i = 1,2,3$; $j = 1,2,3,4,5,6$). These covariants can be simply rewritten from the list of covariants for the group $4_z2_x2_{xy}$ of the preceding paper, because, in this group, vector and pseudovector, tensor δ_{ij} and piezoelectric tensor d_{ij} have the same covariants and **u** is the same in both cases.

From Table 7 and by the use of Tables 4, 5, and 6 we can now deduce the tensorial covariants of: polarization $\mathbf{P} \sim \varepsilon\mathbf{p}$, magnetization $\mathbf{M} \sim \tau\mathbf{p}$, current vector $\mathbf{j} \sim \varepsilon\tau\mathbf{p}$, gyration tensor $\mathbf{g} \sim \varepsilon\mathbf{u}$, symmetric $\boldsymbol{\mu}^S \sim \varepsilon\tau\mathbf{u}$ and antisymmetric $\boldsymbol{\mu}^A \sim \varepsilon\tau\mathbf{p}$ parts of the magnetoelectric tensor $\boldsymbol{\mu}$, piezoelectric tensor $\mathbf{d} \sim \varepsilon\boldsymbol{\delta}$, piezomagnetic tensor $\pi \sim \tau\boldsymbol{\delta}$, and such hypothetical tensors as magnetoconductivity $\varepsilon\mathbf{u} \oplus \varepsilon\mathbf{p}$, electroconductivity $\tau\mathbf{u} \oplus \tau\mathbf{p}$ or piezoconductivity $\varepsilon\tau\boldsymbol{\delta}$ (Ascher, 1966), for all groups of the (oriented) Laue class $4_z2_x2_{xy}$.

Let us, for example, consider the symmetric and antisymmetric parts of the magnetoelectric tensor $\boldsymbol{\mu}$. The first row of Table 8 gives the covariants of $\boldsymbol{\mu}$ for all those groups in which $\varepsilon\tau$ transforms like x_1, *i.e.* for groups $4_z2_x2_{xy}$, $4_zm'_xm'_{xy}$, $\bar{4}'_z2_xm'_{xy}$, and $\bar{4}_zm'_x2_{xy}$. If the covariants are additionally supplied with parity labels $-$, $+$, m, and 1^-_m, they will be relevant to groups $4_z/m_zm_xm_{xy}$, $4_z/m'_zm'_xm'_{xy}$, $4_z2_x2_{xy}1'$, and $4_z/m_zm_xm_{xy}1'$ respectively. The second, third and fourth rows are reorganized according to conversion rules as if the covariants are multiplied by x_2, x_3, and x_4 respectively. Accordingly, the second row gives the covariants for those groups for which $\varepsilon\tau$ transforms like x_2, *i.e.* for groups $4_z2'_x2'_{xy}$, $4_zm_xm_{xy}$, $\bar{4}'_z2'_xm_{xy}$, and $\bar{4}'_zm_x2'_{xy}$ as well as for groups $4_z/m_zm'_xm'_{xy}$, $4_z/m'_zm_xm_{xy}$, and $4_zm_xm_{xy}1'$, where the covariants have to be supplied with parity labels $-$, $+$, and m re-

Table 7. *Covariants of some 1^+_e tensors for Laue class D_4 ($4_z2_x2_{xy}$)*

$\Gamma_1(x_1)$	$\Gamma_2(x_2)$	$\Gamma_3(x_3)$	$\Gamma_4(x_4)$	$R^{(1)}_5(x_5,y_5)$
	p_3			(p_1,p_2)
$u_1 + u_2$ u_3		$u_1 - u_2$	u_6	$(u_4,-u_5)$
$\delta_{14} - \delta_{25}$	$\delta_{31} + \delta_{32}$ δ_{33}		$\delta_{31} - \delta_{32}$	$(\delta_{11},\delta_{22})$ $(\delta_{12},\delta_{21})$ $(\delta_{13},\delta_{23})$
	$\delta_{15} + \delta_{24}$	$\delta_{14} + \delta_{25}$ δ_{36}	$\delta_{15} - \delta_{24}$	$(\delta_{26},\delta_{16})$ $(\delta_{35},\delta_{34})$

Table 8. *Covariants of the magnetoelectricity tensor*

	$\Gamma_1(x_1)$	$\Gamma_2(x_2)$	$\Gamma_3(x_3)$	$\Gamma_4(x_4)$	$R^{(1)}_5(x_5,y_5)$
x_1	$\mu^S_1 + \mu^S_2$ μ^S_3	μ^A_3	$\mu^S_1 - \mu^S_2$	μ^S_6	(μ^A_1,μ^A_2) $(\mu^S_4,-\mu^S_5)$
x_2	μ^A_3	$\mu^S_1 + \mu^S_2$ μ^S_3	μ^S_6	$\mu^S_1 - \mu^S_2$	$(\mu^A_2,-\mu^A_1)$ (μ^S_5,μ^S_4)
x_3	$\mu^S_1 - \mu^S_2$	μ^S_6	$\mu^S_1 + \mu^S_2$ μ^S_3	μ^A_3	$(\mu^A_1,-\mu^A_2)$ (μ^S_4,μ^S_5)
x_4	μ^S_6	$\mu^S_1 - \mu^S_2$	μ^A_3	$\mu^S_1 + \mu^S_2$ μ^S_3	(μ^A_2,μ^A_1) $(\mu^S_5,-\mu^S_4)$

spectively. Analogously, the third and fourth rows give the covariants for those groups in which $\varepsilon\tau$ transforms like x_3 or x_4, without or with parity labels.

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The Joint Probability Distribution of the Structure Factors in a Karle–Hauptman Matrix*

BY J. J. L. HEINERMAN,† H. KRABBENDAM AND J. KROON‡

Laboratorium voor Structuurchemie, Rijksuniversiteit, Padualaan 8, Utrecht, The Netherlands

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Abstract

The joint probability distribution of *all* structure factors $E_{\mathbf{h}_i-\mathbf{h}_j}$ $(i,j = 0, \ldots, m)$ in an $(m+1)\times(m+1)$ Karle–Hauptman matrix is derived for structures in the space group $P1$.

Introduction

The joint probability distribution of the normalized structure factors $E_{\mathbf{h}_0-\mathbf{h}_m}$, $E_{\mathbf{h}_1-\mathbf{h}_m}$, ... and $E_{\mathbf{h}_{m-1}-\mathbf{h}_m}$ where $\mathbf{h}_0, \ldots, \mathbf{h}_{m-1}$ are fixed and $\mathbf{h}_m$ is the primitive random variable leads *via* the conditional joint probability distribution of the phases $\varphi_{\mathbf{h}_0-\mathbf{h}_m}, \ldots, \varphi_{\mathbf{h}_{m-1}-\mathbf{h}_m}$ to the maximum-determinant rule for phase determination: the most probable values for the phases $\varphi_{\mathbf{h}_0-\mathbf{h}_m}, \ldots, \varphi_{\mathbf{h}_{m-1}-\mathbf{h}_m}$ are those for which the determinant of the Karle–Hauptman matrix (Karle & Hauptman, 1950) with last column $E_{\mathbf{h}_0-\mathbf{h}_m}, \ldots, E_{\mathbf{h}_{m-1}-\mathbf{h}_m}, E_0$ takes on its maximum value (de Rango, 1969; Tsoucaris, 1970). The distribution of only one structure factor, say $E_{\mathbf{h}_0-\mathbf{h}_m}$, is obtained by fixing the magnitudes and phases of $E_{\mathbf{h}_1-\mathbf{h}_m}, \ldots, E_{\mathbf{h}_{m-1}-\mathbf{h}_m}$. The maximum of this distribution gives the most probable value for $E_{\mathbf{h}_0-\mathbf{h}_m}$, expressed in (i) the $E_{\mathbf{h}_i-\mathbf{h}_m}$ $(i = 1, \ldots, m-1)$ and (ii) the remaining structure factors in the Karle–Hauptman matrix (de Rango, 1969; Tsoucaris, 1970). From a probabilistic point of view the structure factors (i) and (ii) are of a different nature since for (i) the $E_{\mathbf{h}_i-\mathbf{h}_m}$ are fixed but the reciprocal-lattice vectors $\mathbf{h}_i - \mathbf{h}_m$ are not, while for (ii) the reciprocal-lattice vectors are fixed.

We shall show that it is possible to treat all structure factors in the same way. For structures in space group $P1$ we shall derive the joint probability distribution of *all* structure factors $E_{\mathbf{h}_i-\mathbf{h}_j}$ in a Karle–Hauptman matrix, where all $\mathbf{h}_i$, $\mathbf{h}_j$ are primitive random variables. Two different routes will be followed. The first is straightforward and does not resort to any previous work on determinants. The second involves conditional joint probability distributions and shows both the similarities and differences from the earlier probability calculations that led to the maximum-determinant rule.

As will be shown in the following paper the joint probability distribution of all structure factors in a Karle–Hauptman matrix leads to new functions whose maxima correspond with the most probable values for structure-factor phases.

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† Present address: Koninklijke/Shell-laboratorium, Badhuisweg 3, Amsterdam-N, The Netherlands.
‡ To whom correspondence should be addressed.

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