# **Tensorial Covariants for the 32 Crystal Point Groups**

BY VOJTĚCH KOPSKÝ

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

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## **Abstract**

The recently published tables of Clebsch-Gordan products are applied to derive the tensorial covariants (bases of irreducible or physically irreducible representations) for the 32 crystal point groups. Tensors of the following intrinsic symmetries in Jahn notation are considered:  $\varepsilon$  (pseudoscalar), V (polar vector), [V<sup>2</sup>],  $V[V^2]$ ,  $[V^2]^2$ ,  $[V^2]^2$ ,  $\varepsilon[V^2]$ , and  $\varepsilon V[V^2]$ . With this choice the most important tensors of optical and other properties are covered. Explicit lists of covariants in components of these tensors are given for the noncentrosymmetric groups; with the use of parity arguments the lists also apply to centrosymmetric groups. Applications, especially for phase transitions with reduction of the point symmetry, are briefly discussed.

#### **1. Introduction**

A vast number of original papers and books have already been devoted to practical calculation techniques and to the tabulation of material-property tensors for different magnetic and classical crystal symmetries. The form of the basic physical tensors in equilibrium has already been given for the 32 crystal point groups by Voigt (1910). The contemporary sources usually referenced for the equilibrium form of materialproperty tensors in the classical and magnetic symmetry classes are Nye (1957) and Birss (1964). Zheludev (1964) found the form of the electrogyration tensor, Ranganath & Ramaseshan (1969) gave the tensor of elastogyration, and Smith (1970) tabulated the equilibrium tensors up to the eighth rank. A wide variety of tensor types and their physical interpretation are given by Sirotin & Shaskolskaya (1975). The history of calculation techniques, amongst which the 'direct inspection method' and its modification (Fumi,  $1952a,b$ ) are the most frequently used, can be traced from the referenced sources.

The problem of determining the equilibrium form of a given tensor for a given symmetry group is only part of a more general task to decompose this tensor into bases of REP's (irreducible or physically irreducible representations) of the group in question. For example,

such bases have been dealt with by Fumi  $(1952c)$  who used them to determine, by subductions, the equilibrium form of tensors in subgroups.\* Once the decomposition of a tensor is known we obtain the equilibrium form of a tensor immediately by equating to zero all noninvariant combinations of the tensor components.

The decomposition of second-rank tensors was given by Callen (1968); some tensorial bases of higher rank were considered by Janovec, Dvořák & Petzelt (1975) and also by Zheludev (1976). An inspection of transformation properties or the use of projection operators are the methods usually referenced for achieving the decomposition and the bases are not always specified within the equivalence classes of REP's. As an algebraic problem of finite dimension, the decomposition can always be found in this or some other way. The theory of group representations provides, however, a systematic method which utilizes the Clebsch-Gordan (CG) reduction.

The CG reduction for the 32 crystal point groups is given by Koster, Dimmock, Wheeler & Statz (1963) *via* the CG coefficients. For practical calculations it is more convenient to use tables of the so-called 'CG products' (Kopský, 1976a,b) which give directly the multiplication of bases in the form of bilinear functions. Here we shall apply these tables to derive the tensorial bases of the REP's (or, as we prefer to call them, the tensorial covariants) of the 32 crystal point groups for the main physical tensors up to the fourth rank. The choice of tabulated tensors was governed by a desire to cover all basic optical properties, and continuance to higher ranks, if desired, is straightforward. In the following paper (Kopsky, 1979a) we show how to extend these results in a simple way to all magnetic crystal point groups and to tensors involving magnetic properties.

The terminology which we use here has been described earlier (Kopský, 1976a). The term covariant, originally introduced in a similar context by Weyl (1946), means

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<sup>\*</sup> We owe an apology to Professor Fumi for quoting this work as that of the 'direct inspection method' (Kopský, 1976a). The paper actually deals with a subduction method which makes use of the fact that bases of REP's of a group are connected by subductions with bases of REP's of its subgroups.

the same as the more customary symmetry-adapted basis. Covariants are, however, well defined mathematical objects which form their own linear spaces  $$ this, in my opinion, justifies the revival of Weyls term. The typification of bases, variables and covariants is  $introduced$  here for purposes of standardization  $-$  it is evidently an analogue of the symbolic method in the 'old' theory of invariants (Weitzenböck, 1923).

#### **2. Covariants**

The equivalence classes of REP's of a finite group G of order N are described by characters  $\chi_{\alpha}$  (G),  $\alpha = 1, 2, ...,$  $\kappa$ . In each class  $\chi_{\alpha}$  (G) we can choose one of the equivalent matrix REP's  $\Gamma_{0\alpha}$  (G):  $g \to D^{(\alpha)}$  (g) by assigning to each element g of  $\tilde{G}$  a certain matrix  $D^{(\alpha)}(g)$  of the dimension  $d_{\alpha} = \chi_{\alpha}$  (e). Let A(G):  $g \rightarrow A(g)$  be a representation of G by linear operators  $A(g)$  which act on a carrier space  $\mathsf{L}_n$  and let  $\chi(\mathsf{G})$  be the character of A(G). Then, it is possible to find such bases  $\{e_{\alpha a,i}\}, \alpha = 1, 2,$  $\ldots, \kappa; a = 1, 2, \ldots, n_{\alpha} = (1/N) \sum_{g \in G} \chi(g) \chi^*_{\alpha}(g); i = 1,$ 2, ...,  $d_{\alpha}$ , of the space  $L_n$ , in which:

$$
\mathcal{A}(g)\mathbf{e}_{\alpha a,i} = \mathcal{D}_{ii}^{(\alpha)}(g)\,\mathbf{e}_{\alpha a,i}.\tag{1}
$$

The spaces  $\mathcal{L}_{\alpha a}$ , spanned on  $\{e_{\alpha a,i}\}\ (a, a \text{ fixed})$  are then invariant irreducible subspaces of  $L_n$ . Any nonsingular (and unitary, if orthonormalization of bases is required) transformation  $\zeta: \mathbf{e}'_{\alpha a_i} = \sum_{b=1}^{n a} \zeta_{ab} \mathbf{e}_{\alpha b_i}$  leads to other bases  $\{e'_{\alpha a,i}\}\$  satisfying (1) and to new invariant irreducible subspaces  $\mathcal{L}_{\alpha q}$  of  $\mathcal{L}_{n}$ .

The space  $L_n$  with representation A(G) can be considered as a ground space which produces functional or tensor spaces carrying new (functional or tensor) representations of G defined in an appropriate way. Thus, if  $f(\mathbf{x})$  or  $f(\mathbf{x}, \mathbf{y}, \ldots)$  is a function of one or of several vectors  $x, y \in L_n$ , we can define the action of elements  $g$  of  $G$  on the functions by:

 $\mathscr{A}(g)f(x) = f_{e}(x) = f[A(g^{-1})x],$  (2a)

or

 $\mathscr{A}(g)f(x, y, \ldots) = f_{\mathfrak{g}}(x, y, \ldots)$ 

$$
= f[A(g^{-1}) x, A(g^{-1}) y, \ldots]. \tag{2b}
$$

This definition is common; the transformed functions  $f<sub>e</sub>$ have the same values in the transformed vectors  $A(g)x$ as the original functions f in the original vectors  $x$  and operators  $\mathcal{A}(g)$  form a representation  $\mathcal{A}(G)$  of G.

Particularly, the linear functions of vector  $x \in L_n$ form a linear space  $\tilde{L}_n$ ; one of the possible bases of  $\tilde{L}_n$  is given by the set of functions  $\varphi_{\alpha a,j}$  (x) =  $x_{\alpha a,i}$ , where x  $= x_{\alpha a,i} e_{\alpha a,i}$  Defining operators  $\mathbb{A}(g)$  on  $\mathbb{L}_n$  by (2a), we obtain from (2) and (1):

$$
\tilde{\mathsf{A}}(g) \varphi_{\alpha a,i}(\mathbf{x}) = \varphi_{\alpha a,i}[\mathsf{D}_{kj}^{(\alpha)}(g^{-1}) x_{\alpha a,j} \mathbf{e}_{\alpha a,k}]
$$

$$
= \mathsf{D}_{ij}^{(\alpha)}(g^{-1}) x_{\alpha a,j} = \tilde{\mathsf{D}}_{ji}^{(\alpha)}(g) \varphi_{\alpha a,j}(\mathbf{x}). \tag{3}
$$

The space  $\tilde{\mathsf{L}}_n$ , representation  $\tilde{\mathsf{A}}(G)$ , matrices  $\tilde{\mathsf{D}}^{(\alpha)}(g)$ , and the bases  $\{\varphi_{\alpha a,i}\}\$  are called adjoint to the space  $L_n$ , representation  $\tilde{A(G)}$ , matrices  $D^{(\alpha)}(g)$ , and bases

 ${e_{\alpha a,i}}$ , respectively. An adjoint matrix  $\tilde{D} = (D')^{-1} =$  $(D^{-1})^t$  to a given matrix D is its reciprocal and transposed. In group representation theory we use ordinary unitary matrices; in this case the adjoint matrix  $\tilde{D}$  coincides with the conjugate complex  $D^*$ . If the matrix is also real, *i.e.* orthogonal, then  $\tilde{D}$  and  $D$ coincide.

The functions  $\varphi_{\alpha a,i}$  (*a*, *a* fixed) again span invariant irreducible subspaces  $\mathsf{L}_{\alpha a}$  of  $\mathsf{L}_{n}$  and a nonsingular transformation  $\eta: \varphi'_{\alpha a,i} = \sum_{b=1}^{n} \eta_{ab} \varphi_{\alpha b,i}$  leads<sub>i</sub>to another basis of  $\mathsf{L}_n$ , satisfying (3), and the primed functions span new invariant irreducible subspaces  $\tilde{L}'_{\alpha q}$  of the  $\tilde{L}_{n}$ . If, further, the matrix  $\eta_{ab}$  is adjoint to the matrix  $\xi_{ab}$ , then the primed basis of  $L_n$  is adjoint to the primed basis of  $L_n$ . We say that functions which transform according to (3) form  $\Gamma_{0\alpha}$  covariants. More rigorously, a definition of functional covariants is: A set  $f^{(\alpha)} =$  $(f_{\alpha 1}, f_{\alpha 2}, \ldots, f_{\alpha d_{\alpha}})$  of functions  $f_{\alpha i}$  is called a covariant to the REP  $\Gamma_{0\alpha}(\mathbf{\ddot{G}})$  of the group  $\mathbf{\ddot{G}}$ , or simply a  $\Gamma_{0\alpha}$  covariant, if the functions  $f_{ai}$  are defined on a space  $\mathsf{L}_n$ which carries an operator representation  $A(G)$  of G, if the action of  $\mathcal{A}(g)$  on f, for  $g \in G$ , is defined by  $(2a)$ [or by  $(2b)$  for many argument functions], and if these functions transform among themselves according to:

$$
\mathscr{A}(g) f_{\alpha i} = \tilde{\mathcal{D}}_{ji}^{(\alpha)}(g) f_{\alpha j},\tag{4}
$$

where  $\tilde{D}^{(\alpha)}(g)$  are adjoint to matrices  $D^{(\alpha)}(g)$  of  $\Gamma_{aa}(G)$ . With this definition, the functions  $\varphi_{\alpha a,i}$  form sets  $\varphi_{a}^{(\alpha)}$  $=$   $x_a^{(\alpha)} = (x_{\alpha a,1}, x_{\alpha a,2},...,x_{\alpha a,d})$  – the functions are written explicitly here – which are the linear  $\Gamma_{0\alpha}$  covariants of  $L_n$ .

The following terminology is convenient for the standardization and tabulation of reductions: let the set of chosen matrix REP's  $\Gamma_{0\alpha}(G)$  be a typical matrix representation  $F_0(G)$  of G and let  $\mathbf{x}^{(\alpha)} = (x_{\alpha1}, x_{\alpha2}, \ldots, x_{\alpha n})$  $x_{\alpha d}$ ) be an abstract representative of  $\Gamma_{0\alpha}$  covariants;  $x^{(\alpha)}$  is called the typical  $\Gamma_{0\alpha}$  covariant and its components  $x_{\alpha i}$  are called the typical variables. The reductions of  $\tilde{A}(G)$  and  $L_n$  can be conveniently given as follows:

$$
\Gamma_{0\alpha}(x_{\alpha 1}, x_{\alpha 2}, \dots, x_{\alpha d_{\alpha}})
$$
  
\n
$$
\mathbf{x}_{1}^{(\alpha)} = (x_{\alpha 1, 1}, x_{\alpha 1, 2}, \dots, x_{\alpha 1, d_{\alpha}})
$$
  
\n
$$
\mathbf{x}_{2}^{(\alpha)} = (x_{\alpha 2, 1}, x_{\alpha 2, 2}, \dots, x_{\alpha 2, d_{\alpha}})
$$
  
\n...  
\n
$$
\mathbf{x}_{n}^{(\alpha)} = (x_{\alpha n_{\alpha 1}}, x_{\alpha n_{\alpha 2}}, \dots, x_{\alpha n_{\alpha n} d_{\alpha}}).
$$

To emphasize the fact that this reduction has a specific matrix form  $\Gamma_{0\alpha}$ (G) for each REP, we should say that it is associated with a given typical representation  $\Gamma_0(G)$ . We shall for brevity drop this specification. Analogously we can tabulate the functional covariants.

Covariants have the following useful properties. (i) A

linear combination of  $\Gamma_{0\alpha}$  covariants is again a  $\Gamma_{0\alpha}$ covariant. Hence  $\Gamma_{0\alpha}$  covariants form linear spaces and it is possible to speak about bases of spaces of  $\Gamma_{0\alpha}$  covariants. (ii) If a certain linear relation holds between the jth components of covariants, then the same linear relation holds between all remaining components and therefore between covariants as a whole. (iii) The linear envelope of components of a  $\Gamma_{0\alpha}$  covariant forms an invariant irreducible space, which carries the REP of the class  $\chi_{\alpha}(G)$  – when components of the covariant are taken as a basis, this representation has the matrix form  $\Gamma_{0\alpha}$ (G). (iv) Components of a covariant and components of two linearly independent (particularly those belonging to different REP's) covariants are linearly independent.

The space  $\mathsf{L}_n$  is usually defined by a certain basis  $\{e_i\}$ in which A(G) is not reduced. The problem of finding the basis  ${e_{\alpha a,i}}$  in which L<sub>n</sub> splits into invariant irreducible subspaces  $\mathcal{L}_{\alpha\alpha}$  and A(G) is reduced to the particular matrix form  $\Gamma_{0\alpha}(\mathcal{G})$  on each of  $\mathcal{L}_{\alpha\alpha}$  and the problem of finding  $n_{\alpha}$  linearly independent linear  $\Gamma_{0\alpha}$ covariants on L<sub>n</sub> to each  $\Gamma_{0\alpha}$ (G) are equivalent. Indeed, a vector  $x \in L_n$  can be expressed as either  $x = x_j e_j$  or  $\mathbf{x} = x_{\alpha a_i l} \mathbf{e}_{\alpha a_i l}$ , where  $\mathbf{e}_{\alpha a_i l} = \sum_{j=1}^{n} C_{(\alpha a_i l)} j \mathbf{e}_j$  and  $x_{\alpha a_i l} = i$  $\sum_{i=1}^n d_{(a,q,i);i}x_i$  and the matrices  $c_{(a,q,i);j}$ ,  $d_{(a,q,i);j}$  are mutually adjoint  $(a, i)$  are along the rows, j the columns of c, d]. The linear combinations  $x_{\alpha a,i}$  of original components  $x_i$  are precisely the components of  $n_{\alpha}$  linear  $\Gamma_{0\alpha}$  covariants  $x_{\alpha}^{(\alpha)}$ . If we work with orthonormal bases, then  $c_{(q,q,h)} = d^*_{(q,q,h)}$ ; if the space  $L_n$  is also real, then  $c_{(\alpha a,b)} = d_{(\alpha a,b)}$ . In both cases it is easy to read the bases  ${e_{\alpha a,i}}$  from the table of  $\Gamma_{0a}$  covariants.

# **3. Spaces of tensors and of multilinear functions tensorial covariants**

The classical space of physical vectors is the threedimensional space  $L_3$  spanned on a standard Cartesian basis  $\{e_i\}$ ,  $i = x, y, z$  (or, alternatively  $i = 1,2,3$ ). The metric  $(e_i, e_j) = \delta_{ij}$  defines the scalar product. The full rotation group  $O(3)$  leaves the scalar product invariant. The proper rotations of  $L_3$  form a subgroup  $SO(3)$  of  $O(3)$  and the elements of  $SO(3)$  are specified by their orientation with respect to the Cartesian basis *{ei}* and by the rotation angle. The remaining elements of  $O(3)$ are, in addition, combined with the space inversion  $i$ , which changes the signs of all three vectors  $e_i$ . Thus to each element  $g \in O(3)$  we assign a linear operator  $V(g)$ , which acts on  $e_i$  according to:

$$
\nabla(g)\mathbf{e}_i = \mathbf{D}_{ji}(g)\mathbf{e}_j,\tag{5}
$$

where  $D_{ii}(g)$  are orthogonal matrices. The representation of  $O(3)$  by operators  $V(g)$  is called the vector representation of  $O(3)$ . If we want to work further with absolutely irreducible representations (not with physically irreducible ones), it is necessary to consider  $L_3$  as a space of vectors  $x_i e_i$  with  $x_i$  from the field of complex numbers. Then we can choose a basis  $[(e<sub>x</sub> +$  $i\mathbf{e}_y/\sqrt{2}$ ,  $\mathbf{e}_z$ ,  $(\mathbf{e}_x - i\mathbf{e}_y)/\sqrt{2}$ , in which the vector representation of  $SO(3)$  will have the matrix form denoted usually as  $D^{(1)}$  or, for the full group  $O(3)$ , as  $D^{(1)}$ .

Quite analogously to the previous section we define an adjoint to  $L_3$  space  $\overline{L}_3$  of linear functions on  $L_3$ . The adjoint basis to  $\{e_i\}$  is then formed by the components  $\{x_i\}$  and the adjoint vector representation of  $O(3)$  by operators  $V(g)$  is, because of their orthogonality, expressed by the same matrices as  $\vee$ (g). To the complex basis there will be an adjoint basis  $\frac{x - iy}{\sqrt{2}}$ , z,  $\frac{x + i}{\sqrt{2}}$  $(iy)/\sqrt{2}$ , in which the  $\sqrt{g}$  will be expressed by matrices  $D^{(1)*}$  and  $D^{(1)-*}$  for SO(3) and O(3), respectively.

The k-tuples  $e_{i,j}, \ldots, e_{i}^{(1)}e_{i}^{(2)} \ldots e_{i}^{(k)}$  can be formally accepted as vectors of an orthonormal basis of a  $3<sup>k</sup>$ dimensional space  $L_3^k$ , which has elements:

$$
\mathbf{u} = u_{i_1 i_2 \dots i_k} \mathbf{e}_{i_1 i_2 \dots i_k}.
$$
 (6)

If we also accept that a transformation  $\vee(g)$  of  $\vdash$ , implies the transformation

$$
\bigvee^{k}(g)e_{i_{1}i_{2}\cdots i_{k}}=\bigcup_{j_{1}j_{2}\cdots j_{k}i_{1}i_{2}\cdots i_{k}}^{k}(g)e_{j_{1}j_{2}\cdots j_{k}}\qquad(7)
$$

of  $L_3^k$ , where

$$
D_{j_1j_2...j_k}^k i_{j_1j_2...j_k}(g) = D_{j_1i_1}(g)D_{j_2i_2}(g)...D_{j_ki_k}(g), \quad (8)
$$

then we say that  $\bf{u}$  are the general (asymmetric) tensors of kth rank and  $\vee^k(g)$ ,  $D^k(g)$  are the operators and matrices, in the basis  ${e_{i_1 i_2...i_k}}$  of  $L_3^k$ , of the kth-rank (general) tensor representation of  $O(3)$ .

Again we define an adjoint space  $L_3^k$  with a basis  ${u_{i,i_2...i_k}}$  in which the adjoint operators  $\widetilde{V}^k(g)$  are expressed by the adjoint matrices  $\bar{D}^k(g)$ . This space is a space of linear functions of kth-rank asymmetric tensors. On the other hand, we define a space  $\mathbb{L}_3^k$  of multilinear functions of k vectors  $\mathbf{x}^{(i)} \in L_3$ ,  $i =$ 1, 2, ... k, with a basis  $x_{i_1}^{(1)} x_{i_2}^{(2)} \ldots x_{i_k}^{(k)}$ , on which there act operators  $\tilde{V}^k(q)$  which, in this basis, are expressed by matrices  $\tilde{D}^k(g)$ . We can see almost immediately that the matrices  $\widetilde{D}^k(g)$  and  $\widetilde{D}^k(g)$  would be identical even when the original matrices  $D(g)$  are neither orthogonal nor unitary. Hence there is always a one-to-one correspondence between linear functions of tensor components and multilinear functions of the original vectors given by the correspondence of bases:

$$
u_{i_1 i_2 \ldots i_k} \approx x_{i_1}^{(1)} x_{i_2}^{(2)} \ldots x_{i_k}^{(k)}, \tag{9}
$$

such that the transformation properties of corresponding elements are the same  $-$  the difference between operators  $\sqrt{k}(g)$  and  $\sqrt{k}(g)$  is rather formal. It is more usual to define a tensor by the use of relation (9) as a set of quantities  $u_{i_1i_2...i_k}$  which transform in the same way as the product of  $k$  vector components. The definition of tensor space used here follows the procedure of constructing direct powers in the sense of group representation theory. If we work with the real

basis of the space  $L_3$ , then the original matrices are orthogonal, so are the matrices  $D^k(g)$ , and hence all three matrices  $D^{k}(g)$ ,  $\tilde{D}^{k}(g)$ , and  $D^{k}(g)$  coincide, so that the  $e_{i,i_1,\ldots,i_k}$  also transform as (9).

#### *Intrinsic symmetry*

The tensors of physical properties of crystals are often restricted by requirements of certain symmetry with respect to the permutation of indices  $-$  so-called 'intrinsic symmetry'. Let us recall the results of the theory of representations of the symmetric group  $S_k$  on a kth-rank tensor space (Weyl, 1946; Boerner, 1955; Lyubarskii, 1958): To any permutation

$$
\mathcal{I}_1 = \begin{pmatrix} 1 & 2 & \dots & k \\ 1' & 2' & \dots & k' \end{pmatrix}
$$

of k elements there corresponds an operator  $P(\mathcal{I}_1)$  on the tensor space  $L_3^k$  which transforms the basic tensor  $e_{i,j_1,\ldots,i_k}$  into another basic tensor  $e_{i,j_1,\ldots,i_k}$ . Corresponding matrices are orthogonal and therefore the operators are defined in the same way for the space of functions of tensor components or for the multilinear functions. The most important result of the theory is a consequence of the commutation of operators  $P(\mathcal{I}_1)$ with all operators  $\vee^k(g)$ ; this result is: If S is any subgroup of  $S_k$ , and  $\Gamma_{0\lambda}(S)$  a certain matrix REP of S, then tensors which form the jth component of the  $\Gamma_{0A}(S)$ covariant form an invariant under  $\vee^k(g)$  subspace of  $\mathcal{L}_3^k$ .

Intrinsic symmetries are particular cases of permutational symmetries; they require either that a tensor does not change under certain permutations or that it changes its sign. It means that intrinsic symmetry is characterized by identity or by alternating REP of a certain subgroup S of  $S_k$ . The Jahn symbols for intrinsic symmetries are well known (Jahn, 1949; Sirotin & Shaskolskaya, 1975). If we label the intrinsic symmetry  $\lambda$ , then kth-rank tensors of intrinsic symmetry  $\lambda$  form an invariant under  $\forall^{k}(g), g \in O(3)$ , subspace  $\mathsf{L}_{3,1}^k$  or  $\mathsf{L}_3^k$ . Accordingly, the tensor representation restricted to this subspace should be additionally labelled by  $\lambda: \vee_{\lambda}^{k}$ . In practice we use the customary notation  $[\mathbf{V}^2], {\mathbf{V}^2}, \mathbf{V}[\mathbf{V}^2],$  *etc.* 

## *Tensorial covariants*

Any crystal point group  $G$  is a subgroup of  $O(3)$ . If we have the kth-rank tensor representation  $\vee_A^k$  of intrinsic symmetry  $\lambda$  for the group  $O(3)$ , then by selecting only operators  $\vee_A^k(g)$ ,  $g \in G$ , we get the kthrank tensor representation of intrinsic symmetry  $\lambda$  for the group G. This restriction is called subduction and the representation is denoted  $\vee_3^k(G) = \vee_3^k \downarrow G$ ; it operates on the same space  $L_{31}^{k}$ . For simplicity we denote the basic vectors  $\{e_i\}$  of  $\mathcal{L}_{3\lambda}^k$  by the single index *i*. Then the tensor  $\mathbf{u} \in L_{3\lambda}^k$  is simply a linear combination  $\mathbf{u} = u_i \mathbf{e}_i$ . Let  $\Gamma_{0\alpha}(\mathcal{G})$  be the chosen matrix REP's of the group G

which compound its typical matrix representation. Then the definition of the tensorial covariant is: The linear  $\Gamma_{0\alpha}$  covariant on  $L_{3\lambda}^k$  is called the tensorial  $\Gamma_{0\alpha}$  covariant of the kth rank and of intrinsic symmetry  $\lambda$ .

The number of linearly independent tensorial covariants can be simply calculated by the orthogonality theorem for the characters. The jth component of such a  $\Gamma_{0\alpha}$  covariant is a linear combination  $u_{\alpha a,j} = c_{(\alpha a,j)i}u_i$ and finding the covariants means the same as finding the bases  $e_{\alpha a,i} = c_{(\alpha a,i)i}e_i$ , in which the tensor representation  $\vee_{\lambda}^{k}$  (G) is reduced to a form prescribed by the typical matrix representation of G.

# **4. The Clebsch-Gordan products**

Let  $A_{\alpha}(G)$ ,  $A_{\beta}(G)$  be operator representations of G acting on invariant irreducible subspaces  $L_{0,\alpha}$ ,  $L_{0,\beta}$  and let these be, in the bases  ${e_{\alpha i}}$ ,  ${e_{\beta i}}$  of  $L_{0\alpha}$ ,  $L_{0\beta}$ , expressed by the matrix REP's  $\Gamma_{0\alpha}(\mathcal{G})$ ,  $\Gamma_{0\beta}(\mathcal{G})$  of the fixed typical matrix representation  $\Gamma_0(G)$ . The direct product  $A_{\alpha\beta}(G) = A_{\alpha}(G) \otimes A_{\beta}(G)$  of REP's acts on the direct product  $L_{\alpha\beta} = L_{0\alpha} \otimes L_{0\beta}$  of spaces and, in the basis  $\{e_{\alpha i}e_{\beta j}\}\$  of  $L_{\alpha \beta}$ , the operators are expressed by matrices of the direct product  $\Gamma_{0\alpha}(\mathcal{G}) \otimes \Gamma_{0\beta}(\mathcal{G})$ . The representation  $A_{\alpha\beta}$  (G) contains a REP of a class  $\chi_{\alpha}$  (G) just  $(\alpha \beta \mu) = (1/N) \sum_{g \in G} \chi_{\alpha}(g) \chi_{g}(g) \chi_{\alpha}^{*}(g)$  times and it is therefore possible to find just  $(\alpha\beta\mu)$  invariant irreducible subspaces  $\mathcal{L}_{um}$  of  $\mathcal{L}_{\alpha\beta}$ , and bases  $\{E_{um,k}\}\$ ,  $m \equiv$ 1,2,...,  $(\alpha \beta \mu)$ ;  $k = 1, 2, ..., d_{\mu}$ , in which  $A_{\alpha \beta}(G)$  has the matrix form  $\Gamma_{0\mu}(\mathbb{G})$  prescribed by the typical representation. These bases must be linear combinations of  $e_{\alpha i}e_{\beta j}$ :

$$
\mathbf{E}_{\mu m,k} = \sum_{i,j} (\alpha i \beta j) \mu k \,_{m} \, \mathbf{e}_{\alpha i} \, \mathbf{e}_{\beta j}, \tag{10}
$$

where  $\left(\alpha i \beta j \mu k\right)_{m}$  are the Clebsch-Gordan coefficients which form the transformation matrix from the basis  $\{e_{\alpha i}e_{\beta j}\}\)$  to the basis  $\{E_{\mu m,k}\}\$ .

The use of adjoint spaces is more convenient, especially for tabulation. Here we have two typical covariants  $x^{(\alpha)}$  and  $x^{(\beta)}$ , whose components form bases of invariant irreducible spaces  $\tilde{L}_{0\alpha}$ ,  $\tilde{L}_{0\beta}$ . There then exist  $(a\beta\mu) \Gamma_{0\mu}$  covariants of the form:

$$
\varphi_{\mu m,k} = \sum_{i,j} (\alpha i \beta j | \mu k)^*_{m} x_{\alpha i} x_{\beta j}, \qquad (11)
$$

bilinear in  $x_{ai}$ ,  $x_{aj}$  and linearly independent. The components of these covariants span invariant irreducible subspaces  $\tilde{L}_{\mu m}$ , of the direct product space  $\mathcal{L}_{0\alpha} \otimes \mathcal{L}_{0\beta}$ . We call these covariants the Clebsch-Gordan products of covariants  $x^{(\alpha)}$  and  $x^{(\beta)}$ . Having these products for all pairs of covariants, we can perform reduction of a direct product of any two spaces  $L_n$ ,  $L_m$ , provided that the spaces  $L_n$ ,  $L_m$  are already reduced. Indeed, the reduction of  $\mathsf{L}_n$ ,  $\mathsf{L}_m$  can be given by sets of covariants  $x_a^{(\alpha)}$ ,  $x_b^{(\beta)}$ , respectively, while the

reduction of the direct product space  $L_n \otimes L_m$  is given by their CG products, which can be easily found by formula (11). Thus the products of typical covariants give the prescription for multiplying any particular covariants. I gave this prescription for all magnetic crystal point groups (Kopský, 1976b) and shall now use it to derive tensorial covariants.

The use of CG products in tensor calculus is based on the similarity of transformation properties of tensors and of multilinear functions (9). We can, by consecutive use of CG products, find multilinear covariants as well as covariants of kth-rank asymmetric tensors. Tables of CG products also describe symmetrization in two indices and can be used (as we shall see in practice in §5) to calculate directly those tensors which are obtained by direct multiplication and symmetrization in two indices. Generally (as, for example, in the case of fully symmetrized or antisymmetrized tensors of rank higher than two), we have to perform the symmetrization as an additional procedure. Such cases are not treated here; in particular cases, the symmetrization can be performed without problems. A quite general theory of tensorial covariants is connected with the theory of polynomial and multilinear covariants which is being developed.

# **5. Tensorial covariants for the 32 crystal point groups**

In Appendix I the list of tensors is given, and then lists of their covariants for crystal point groups are given in Appendix II. The covariants are given as linear combinations of tensor components with respect to a standard Cartesian frame of reference and their form depends, for a given group, on the orientation of the group and on the choice of its typical representation. We shall associate the covariants here with the same typical representations as those used in lists of CG products. Of the two schemes given in Kopsky  $(1976b)$ the real one is used, so that the covariants in the present paper are real. The requirements of reality and irreducibility are, however, not compatible for cyclic groups and for groups  $T$ ,  $T_h$ . These groups have onedimensional complex REP's which appear in mutually conjugate complex pairs. As usual, we join such pairs into one REP and bring it to a real form known as a physically irreducible representation (a representation irreducible in the real field but reducible in the complex one). It follows that if  $(x, y)$  is a covariant to such a REP, then  $(y, -x)$  is also a covariant to the same REP. Of these two covariants only one is given.

# **6. Orientation of groups and choice of typical representations**

The lists of covariants (Appendix II) are divided into 11 Laue classes (Henry & Lonsdale, 1952). The orientation of the proper rotation groups which determine the Laue classes is chosen in the usual way: the unique axis is along the z direction and one of the auxiliary axes is along the  $x$  direction; the cubic axes of cubic groups are along the *x,y,z* directions. The noncentrosymmetric groups of a given Laue class are isomorphous with the proper rotation group and have, therefore, the same system of REP's. Groups with the same orientation as the proper rotation group are chosen; in cases when there are two such groups in the same crystal class the covariants are given explicitly for only one. The noncentrosymmetric groups then have, apart from the space inversion, the same elements as the proper rotation group. The matrix REP  $\Gamma_{0\alpha}(\mathcal{G})$  of the proper rotation group assigns to an element  $g \in G$  a matrix  $D^{(\alpha)}(g)$ ; in a noncentrosymmetric group there again corresponds to g either g or *ig;* to this element is again assigned the matrix  $D^{(\alpha)}(g)$ . The orientation of the centrosymmetric group  $G_h = G \times I$  is defined by the orientation of its proper rotation subgroup. The number of REP's of  $G_h$  is twice that of G and we distinguish them by parity labels + or  $-$  (g or u in spectroscopic notation) which indicate whether the matrix of  $i$  is the unit matrix or its negative. The numerical labels of REP's and the choice of matrices for proper rotation elements are the same as for the proper rotation group.

The tensorial covariants are arranged in lists common for all groups of the (oriented) Laue class. The first row of each list contains the REP's in the  $\Gamma$ notation and a set of typical variables (the typical covariant) follows the  $\Gamma$  symbol. The covariants of odd space parity tensors are given in rows for the noncentrosymmetric groups, which are specified at the left-hand side of each row by the international symbol with indices denoting the orientations of the elements. The columns specify the types of covariants. The covariants of even space parity tensors are common for all noncentrosymmetric groups, because these tensors are insensitive to the space inversion (and because of the choice of REP's for the noncentrosymmetric groups). They are given in the lowest row of each list and designated as common or, for groups  $C_3$  and T, which have no noncentrosymmetric isomorphs, as even.

As concerns the numerical labels, the covariants for the centrosymmetric group are, because of the choice of REP's, the same as for the proper rotation group; additionally, they have to be supplied by parity  $+$  or  $$ according to whether the tensor is even or odd. The covariants of the centrosymmetric group can therefore be found in the row for the proper rotation group if the tensor is odd, and in the row common (or even) if the tensor is even.

To correlate our  $\Gamma$  labelling of REP's with the usual spectroscopic notation (Heine, 1960) we give, below each list, the correspondence of typical variables to spectroscopic symbols.

# **7. Derivation of tensorial covariants**

For the vector which is represented by polarization  $P = (P_1P_2, P_3)$ ,  $(x, y, z \sim 1, 2, 3)$  and for pseudoscalar  $\varepsilon$ we have to determine transformation properties by inspection. In the choice of matrix REP's, the use of tensor calculus has been anticipated, so that the correspondence of  $P_i$ , to typical variables is seen almost at once. The pseudoscalar belongs to the identity REP of the proper rotation group and to the  $\Gamma_1^-$  REP of the centrosymmetric group. For a noncentrosymmetric group,  $\varepsilon$  belongs to that one-dimensional alternating REP  $\Gamma_{\alpha}$  which has characters  $-1$  for those elements which are combined with the space inversion. Hence  $\varepsilon$ transforms, in such a group, as  $x_{\alpha}$ .

With lists of CG products at hand, the rest of the work is routine. First we write the  $P_i$  and  $\varepsilon$  under that typical variable which transforms in the same way; we do the same with other tensors as we proceed with the calculation. For higher-rank tensors, the CG products often yield sets of covariants which can be replaced by their linear combinations of simpler form. We proceed consecutively from tensors of lower rank to tensors of higher rank using the similarity of the transformation properties of components of higher-rank tensors with bilinear combinations of components of pairs of lowerrank tensors.

Thus the symmetric second-rank tensor  $u_{ik}$  transforms as the symmetric combination  $(P_i P'_k + P_k P'_i)$ . In the lists we use the usual abbreviated notation:  $u_1 =$  $u_{xx}$ ,  $u_2 = u_{yy}$ ,  $u_3 = u_{zz}$ ,  $u_4 = 2u_{yz}$ ,  $u_5 = 2u_{zx}$ ,  $u_6 = 2u_{xy}$ . To determine the piezoelectric covariants, we recall that  $d_{ik}$  transforms like  $P_i u_k$  ( $i = 1, 2, 3; j = 1, 2, 3, 4, 5, 6$ ). The elastic tensor  $s_{ik}$  transforms as the symmetric combination  $(u_i u'_k + u_k u'_i)$ , the gyration tensor  $g_{ik}$  like  $\epsilon u_{ik}$ , and the tensor of electrogyration  $A_{ik}$  like  $\epsilon d_{ik}$ . The last tensor here for which the covariants are given is the elastogyration tensor  $Q_{ik}$  which transforms like  $u_i u_k$ (the asymmetric square of tensor u). To save space I use the fact that Q can be decomposed into its symmetric part (1/2)  $(Q_{ik} + Q_{ki})$  which transforms like  $s_{ik}$  and into its antisymmetric part  $q_{ik} = (1/2) (Q_{ik} - Q_{ik})$  $\hat{Q}_{ki}$ ) which transforms like  $(u_iu'_k - u_ku'_i)$ . In certain cases the q covariants are the same as the s covariants; this is indicated in the lists by an asterisk at the s covariant. However, sometimes the indices of components in the q covariant are reversed as compared with those of the corresponding s covariant (this is because  $s_{ik}$  is symmetric while  $q_{ik}$  is antisymmetric and that we always used the smaller index of s as the first one). The necessity of reversing the indices for the q covariant is indicated by underlining the indices of the component  $s_{ik}$ . Several q covariants cannot be expressed in this way and these are given separately.

Performing the calculations for each group and collecting the results into lists as described, we can observe a certain regularity with which the odd parity covariants change as we pass from the proper rotation group to its noncentrosymmetric isomorphs. This regularity is due to the following: If a certain linear combination of components of a tensor of odd parity transforms as  $x_{ai}$  for the proper rotation group, then the same combination must transform in a noncentrosymmetric group as  $\epsilon x_{\alpha i}$ . Below the lists of covariants I indicate the effect that multiplication by  $\varepsilon$  has on transformation properties of typical variables for all noncentrosymmetric groups of a corresponding (oriented) Laue class. In the following paper I shall consider analogous relations more closely with the aim of simplifying the calculation of tensorial covariants for magnetic point groups.

## **8. Some applications**

## (i) *Equilibrium form of tensors*

Properties of a physical system in equilibrium must be invariant under the operations of its symmetry group, while the noninvariant properties must vanish. The invariant combinations of tensor components are given in the column of invariants; equating all other covariants to zero we obtain a set of conditions which the equilibrium tensor components have to satisfy. These conditions are given in brackets in the column of invariants.

#### (ii) *Phenomenology of struetural phase transitions*

The components of tensorial covariants mean physically the fluctuations and are important in the consideration of structural phase transitions with change of point symmetry. If we find covariants from components of homogeneous modes, then we can say what mode contributes to what tensorial property. The Landau transition parameter means in our language the set of components of a covariant. We can see from the tables that, apart from transitions that are driven by polarization or by deformation (ferroelectric and ferroelastic transitions) there are also conceivable transitions in which material tensors play macroscopically the role of the transition parameter; the lowest tensors connected with such transitions are  $d$ ,  $g$ , and  $A$ . The 'gyrotropic phase transitions', in which the optical rotatory power is the sole property accompanying the transitions or in which the tensor g acquires new components in the low-symmetry phase, deserve attention and have been studied with the use of the lists presented here (Koňák, Kopský & Smutný, 1978). One example of such a transition has already been reported in caesium cupric chloride,  $CuCsCl<sub>3</sub>$  (Hirotsu, 1975). As long as we work only with the 32 classical groups, we can consider only those transitions which do not involve magnetic properties. We can, evidently, expect that new (so-far unconsidered) phase transitions can be predicted from an inspection of tensorial covariants for the magnetic point groups.

As a minor application, let us mention the possibility of reading directly from the tables the switching forces for ferroelastoelectric and ferrobielastic domains (Cross & Newnham, 1974). The former are given by the components of the piezoelectric tensor  $d_{ik}$  which can be replaced by a combination  $E_i \sigma_k$  of the external electric field  $E$  of external stress  $\sigma$ , the latter by components of the elastic tensor  $s_{ik}$  which can be analogously replaced by the combination  $\sigma_i \sigma_k$ .

Phase transitions can be studied globally as relations between a group and its subgroup by the use of typical variables as representatives of physical parameters. The advantage of such an approach is clear; the number of relations which have to be considered is sharply reduced. I have found that out of about one thousand physically different transitions from magnetic point groups (except paramagnetic groups  $C'_{4h}$ ,  $C'_{6h}$ ,  $D'_{2h}$ ,  $D'_{4h}$ ,  $D'_{6h}$ ,  $T'_{h}$ , and  $O'_{h}$ ) to their subgroups there are only 44 abstractly different types. The domain and finedomain structures have been determined for these types  $(K$ opský, 1979b) as well as the corresponding thermodynamic potentials. To transfer these abstract results to the physical interpretation the typical variables need to

be correlated with their actual meaning in individual cases, as is done in the lists of covariants.

# **APPENDIX I List of tabulated tensors**



Several relations between tensors:

$$
\mathbf{u} \sim [\mathbf{P} \otimes \mathbf{P}], \mathbf{d} \sim \mathbf{p} \otimes \mathbf{u}, \mathbf{s} \sim [\mathbf{u} \otimes \mathbf{u}], \mathbf{Q} \sim \mathbf{u} \otimes \mathbf{u}, \mathbf{g} \sim \varepsilon \mathbf{u}, \mathbf{A} \sim \varepsilon \mathbf{d}.
$$
  
\n
$$
\mathbf{Q} = \mathbf{Q}^{\text{sym}} + \mathbf{Q}^{\text{antisym}}, \quad Q^{\text{sym}}_{ij} = (1/2)(Q_{ij} + Q_{ji}),
$$
  
\n
$$
q_{ij} = Q^{\text{antisym}}_{ij} = (1/2)(Q_{ij} - Q_{ji}).
$$
  
\n
$$
Q^{\text{sym}}_{ij} \sim s_{ij}.
$$
  
\nThe symbol  $\sim$  means transforms like.

# **APPENDIX II**

#### **Tensorial covariants for the 21 noneentrosymmetrie and 11 eentrosymmetrie crystal point groups**

All odd tensor components are  $\Gamma_1^-$  covariants  $(\Gamma_1^- - A_\nu)$  and are forbidden in equilibrium.

Triclinic, monoclinic and orthorhombic point groups Laue class  $C<sub>1</sub>$ 



Laue class  $C_2$ 



Laue class  $D_2$ 

	$\Gamma_1(x_1)$	$\Gamma_2(x_2)$	$\Gamma_3(x_3)$	$\Gamma_4(x_4)$
$D_2(2_x 2_y 2_z)$	$g_1$ $g_2$ $g_3$ ε	$P_3$ $g_6$ $d_{31}$ $d_{32}$ $d_{33}$	$P_1$ $g_4$ $d_{11}$ $d_{12}$ $d_{13}$	$P_2$ $g_5$ $d_{21}$ $d_{22}$ $d_{23}$
	$d_{14}$ $d_{25}$ $d_{36}$	$d_{15}$ $d_{24}$	$d_{26}$ $d_{35}$	$d_{16}$ $d_{34}$
$C_{2\nu}$ $(m_x m_y 2_z)$	$P_3$ $g_6$	$g_1$ $g_2$ $g_3$ ε	$P_2$ $g_5$	$P_1$ $g_4$
	$d_{31}$ $d_{32}$ $d_{33}$ $d_{15} d_{24}$	$d_{14}$ $d_{25}$ $d_{36}$	$d_{21}$ $d_{22}$ $d_{23}$ $d_{16} d_{34}$	$d_{11}$ $d_{12}$ $d_{13}$ $d_{26}$ $d_{35}$
Common	$u_1$ $u_2$ $u_3$	$u_{6}$	$u_4$	$u_{5}$
	$S_{11}$ $S_{22}$ $S_{33}$	$S_{16}$ $S_{26}$ $S_{36}$	$S_{14}$ $S_{24}$ $S_{34}$	$S_{15}$ $S_{25}$ $S_{35}$
	$S_{12}$ $S_{13}$ $S_{23}$	$\boldsymbol{S_{45}}$	$s_{56}$	$s_{46}$
	$S_{44}$ $S_{55}$ $S_{66}$	$A_{31}A_{32}A_{33}$	$A_{11}A_{12}A_{13}$	$A_{21}A_{22}A_{23}$
	$A_{14}A_{25}A_{36}$	$A_{15}A_{24}$	$A_{26}A_{35}$	$A_{16}A_{34}$
	$x_1, x_2, x_3, x_4$	$\varepsilon$ [ $x_1$ , $x_2$ , $x_3$ , $x_4$ ]		
$D_2(2_x2_y2_z)$	$A, B_1, B_3, B_2$	$x_1, x_2, x_3, x_4$		
$C_{2\nu}$ $(m_x m_y 2_z)$	$A_1, A_2, B_2, B_1$	$x_2, x_1, x_4, x_3$		
$C_{2\nu}(m_x 2, m_z)$		$x_4, x_3, x_2, x_1$		

 $x_3, x_4, x_1, x_2$ 

# Tetragonal point groups

Laue class  $C_4$ 

 $C_{2\nu} (2_x m_y m_z)$ 



 $\hat{\mathcal{A}}$ 

 $\hat{\mathcal{A}}$ 

Laue class  $D_4$ 



 $D_{2d}$  (4<sub>z</sub>m<sub>x</sub>2<sub>xy</sub>)  $x_4, x_3, x_2, x_1, (y_5, x_5)$ 

#### Trigonal and hexagonal point groups Laue class  $C_3$





Laue class  $D_3$ 



 $C_6(6z)$  *A*, *B*,  $E_2$ ,  $E_1$  $C_{3h} (6, 0, 0, A', A'', E', E'')$  $x_1, x_2, (x_5, y_5), (x_6, y_6)$  $x_2, x_1, (x_6, y_6), (x_5, y_5)$ 

Laue class  $D_6$ 



 $\mathcal{L}^{\pm}$ 

Cubic point groups

**Laue class T** 





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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 (symmetryadapted tensorial bases) of even parity with respect to

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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  $D<sub>4</sub>$ .

# **1. Introduction**

In the preceding paper (Kopsky, 1979) it has been shown how to find tensorial covariants with the help of standard tables of Clebsch-Gordan products (Kopský, 1976a, 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 © 1979 International Union of Crystallography