Acta Crystallographica Section A
Foundations of Crystallography
ISSN 0108-7673

Received 19 August 2005
Accepted 6 January 2006

Application of modern tensor calculus to engineered domain structures. 1. Calculation of tensorial covariants

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This article is a roadmap to a systematic calculation and tabulation of tensorial covariants for the point groups of material physics. The following are the essential steps in the described approach to tensor calculus. (i) An exact specification of the considered point groups by their embellished Hermann–Mauguin and Schoenflies symbols. (ii) Introduction of oriented Laue classes of magnetic point groups. (iii) An exact specification of matrix ireps (irreducible representations). (iv) Introduction of so-called typical (standard) bases and variables – typical invariants, relative invariants or components of the typical covariants. (v) Introduction of Clebsch–Gordan products of the typical variables. (vi) Calculation of tensorial covariants of ascending ranks with consecutive use of tables of Clebsch–Gordan products. (vii) Opechowski's magic relations between tensorial decompositions. These steps are illustrated for groups of the tetragonal oriented Laue class $D_{4z} - 4_z 2_x 2_{xy}$ of magnetic point groups and for tensors up to fourth rank.

1. Symmetry and material properties

The physical properties of materials are in a certain manner connected with their symmetry. This relationship between symmetry and properties is expressed by principles that bear the names of Neumann (1885), Curie (1884*a*,*b*) and, in the russian literature, also of Minnigerode (1887). Neumann's principle is usually applied for consideration of tensor properties in a form that says that *the property must be invariant under symmetry operations of the material*. Though the statement is true, it can be easily misinterpreted. Its weakness becomes clear if we realize that the symmetry of each particular property itself contributes to our knowledge of the symmetry of the material. Usually we assume that our material is an ideal crystal and we know the symmetry from measurements of its structure, though at the time when the principle was formulated the symmetry was deduced from the external shape of monocrystals. As a classical example of misunderstanding, we can name the concept of the *cubic ferromagnet*, which appears in the older literature on magnetic garnets. X-ray analysis of these crystals leads to the conclusion that their symmetry is cubic, which is incompatible with the existence of magnetism. More precise measurements later showed that the structure of these crystals in the magnetic state slightly deviates from cubic due to magnetostriction.

To avoid misinterpretations of this type, it is worth realizing that conclusions about symmetry can be made from measurements of any of the properties and that the measurement of any property may give incomplete information about the symmetry. It is probably best to formulate the relationship between properties and symmetry as follows.

If, by measuring any property of a crystal, we find that the symmetry of this property is a certain point group G, then the symmetry of the crystal cannot be higher than G.

In other words, if we measure different properties, including the structure, we can conclude from such measurements only that the symmetry of the crystal (or other material) is not higher than the intersection of the symmetries of these properties. On the other hand, the symmetry of a certain property can be higher than the symmetry of the material. Again we have the classical example of the optical indicatrix (or dielectric constant) whose symmetry is the maximal cubic group $O_h = m\bar{3}m$ in crystals of any lower cubic symmetry.

The origin of such discrepancies as the case of the cubic ferromagnet lies in the fact that the precision of any physical measurement is limited so that we are never able to say about a measurement in physics that it is exact. External shape and structural analysis are usually sufficient to draw conclusions about symmetry but we cannot consider them as absolute criteria as shown by the example of the cubic ferromagnet.

With this in mind, we may, however, use the usual routine to connect tensorial properties with the symmetry. There is nothing wrong in concluding that the allowed tensor properties of a crystal are those that are invariant under its point symmetry G. If, contrary to this, we find experimentally some tensorial property that is not invariant under this group, we conclude that the actual symmetry must be lower. As long as we are not able to detect such deviation, we may safely assume that the symmetry is G.

Another point of our consideration is connected with the notion of the *point group*. According to terminology that is accepted by *International Tables for Crystallography*, the term point group G means the factor group of the space group $\mathcal{G}$ by its translation subgroup T_G and this group acts on the vector space $V(3)$ associated with the Euclidean space $E(3)$. Since crystals (and other materials) are objects in $E(3)$, the point group in this meaning cannot technically be applied to them. The main objectives of our considerations are the *ferroic phase transitions*, *i.e.* transitions denoted by $G \Downarrow \{F_i\}$ in which the point symmetry of a crystal decreases from G to one of the set of conjugate subgroups F_i (or to a normal subgroup H) and, as a result, some new tensor properties onset which were not allowed by the *parent symmetry G* (*cf.* Kopský, 2006*b*, hereafter denoted paper 2). Point groups are practically used in all papers concerning these transitions which is in contradiction with their interpretation as factor groups of the space groups. There are two possible models and interpretations.

1. We assume that the crystal is small so that we can represent it as a point P in the space $E(3)$. In this case, the symmetry of the parent phase is to be considered as the *site point group* G_P and the symmetry of an individual domain in the ferroic phase as that of one of the site point groups F_{Pi}. This, however, contains an assumption that the whole crystal in the ferroic phase has the same symmetry and hence this approach can be applied only to a single domain state.

2. We adopt the model of an ideal crystal that fills the whole space and consider it in the continuous approximation. In this case, we should consider the parent symmetry as the *point-like space group VG* (Kopský, 2006*c*) and the ferroic symmetries as the point-like space groups $V\{F_i\}$. Instead of tensors, we should consider homogeneous tensor fields on which these groups act. As long as we are interested only in conclusions about new tensor properties in ferroic states, we may abbreviate our results by considering point groups and tensors, bearing the actual meaning in mind. However, once we start studying the distinction of domain pairs and the properties of domain walls, we have to switch our language to that of point-like space groups and tensor fields. The symmetries of domain walls should then be interpreted as the point-like layer groups and the problem to be solved is to find the changes of domain fields as we go from one domain to the other across the domain wall.

As always in applications of group theory, symmetry can predict only which effects are allowed but not their magnitude. Voigt (1910) was the first to calculate allowed tensor properties and his work was followed by the publication of numerous methodical papers. Nowadays information concerning allowed tensor forms is available in several recognized textbooks of which we name Nye (1957), Wooster (1973), Sirotin & Shaskolskaya (1975), Shuvalov (1988), magnetic properties are considered by Birss (1964) and the last but not least source is the very recent Vol. D: *Physical Properties of Crystals* of *International Tables for Crystallography* (2003), where references to the original literature are also given. The methods of calculation such as 'direct inspection' are close to a 'brute force' use of linear algebra. Consideration of group isomorphisms, direct products with inversions together with tensor parities facilitates a more systematic approach.

The material for this paper goes back to rather old investigations by the author which resulted in group-theoretical techniques tailored for calculation of tensorial and polynomial bases of ireps (irreducible representations) and of their use in consideration of ferroic phase transitions. These investigations were motivated by the theory of structural phase transitions in which we need to know tensorial bases of ireps of the parent groups. For tensors up to second rank such bases were given by Callen (1968) and Callen *et al.* (1970). The first attempt to calculate these bases for higher ranks by Janovec *et al.* (1975) was based on the tedious method of projection operators (Tinkham, 1964) and was motivated by the need to find bases for all nonmagnetic ferroic phase transitions.

Our approach described below in detail is based on the method of *Clebsch–Gordan products* in terms of *standard typical variables*, which are representatives of all quantities that transform in a well defined way under the action of considered groups (Kopský, 1976*a*,*b*). By use of this method, we derived tensorial covariants (bases of irreducible representations) for tensors up to fourth rank (Kopský, 1979*a*) for nonmagnetic cases and we have shown how to extend the results to magnetic groups and properties (Kopský, 1979*b*). Later we realized that the calculations are drastically simplified by using relations to which we gave the name *Opechowski's magic relations* (Kopský, 2006*a*) in honour of the late Professor Opechowski who inspired this line of reasoning by observing a certain relationship between the form of tensors of the same intrinsic symmetry but of different parities in different magnetic point groups (Opechowski, 1975; see also Ascher, 1975). This relationship was explained by Kopský (1976*c*) and used by Grimmer (1991) to relate forms of different tensors in different groups. We shall close this paper with an example of the decomposition of related tensors in related groups.

Our latest results concern the distinction of domain states in their tensor properties which is particularly applicable to the newly developing subject of domain engineering. Experience with these calculations has shown that it is desirable to introduce and fix standard choices and symbols of point groups and of their irreducible representations. Our main philosophy is that even the symbols should bear as much information as possible. None of the existing notations, including those used originally by this author, meets the requirements of consistency and transparency of existing relations to the same extent as the standards proposed in this work.

A complete and unified system of symbols for representative point groups and typical variables was used for the derivation of the tables which describe symmetry descents in terms of classical point groups. These tables are now available in printed form (Kopský, 2001) and the whole scheme, supplemented by exact tables of equitranslational subgroups of the space groups, is the main subject of a software supplement *GI ⋆ KoBo-1* (*Group Informatics*, release 1) to Vol. D of *International Tables for Crystallography* (Kopský & Boček, 2003). These two sources also contain a comparison of our symbols of symmetry operations and of ireps with those used by other authors. From the comparative tables of notations, one can really see the necessity to introduce our own, internally compatible, standard notation.

The paper is divided into two parts. In the current part, we shall describe the scheme that facilitates the decomposition of tensors into tensorial covariants (bases of ireps). It will be shown in the second part how to utilize the results for the analysis of tensorial properties of multidomain systems.

2. Introduction to our standard notation for specific point groups

Tensor properties are usually expressed with reference to a certain orthonormal (Cartesian) basis ($\mathbf{e}_x, \mathbf{e}_y, \mathbf{e}_z$) of the vector space $V(3)$. It is therefore also necessary to specify the orientation of the point group G to consider its action on any given tensor. Once the orientation of a point group G is specified, the space of its tensorial invariants (and hence the allowed form of tensors) is unambiguously determined. To define unambiguously the decomposition of tensors into tensorial covariants, it is also necessary to specify matrix ireps of the point group G. This will be done in §6. Here we begin with the specification of symbols for symmetry operations with reference to the Cartesian basis.

Group elements: It is sufficient for our purposes to consider only the elements of specifically oriented groups of the geometric classes $O_h - m\bar{3}m$ and D_{6h}. For the group O_h, we choose the natural orientation where the fourfold axes are oriented along the basis vectors ($\mathbf{e}_x, \mathbf{e}_y, \mathbf{e}_z$) of the Cartesian system. For the group $D_{6h} - 6_z/m_z m_x m_y$, we choose one of the twofold axes along the vector $\mathbf{e}_x$ and the hexagonal axis along the vector $\mathbf{e}_z$. Since there is no possibility of misunderstanding, we shall use the same symbols for the cubic groups and Schoenflies symbol for the group D_{6h} as for the corresponding geometric classes. Let us observe that the two groups in the above-mentioned orientations have in common exactly the group $D_{2h} - m_x m_y m_z$ for which we again use the same Schoenflies symbol as for the whole geometric class.

The elements of these two groups are denoted by symbols that shall be further referred to as the *Standard notation*. The principle of this notation is quite commonly used in the literature and it also coincides with the principle on which the recent proposal of a nomenclature in higher dimensions (Janssen *et al.*, 2002) is based. Rotations about axes of angles π, $2\pi/3$, $\pi/2$ and $\pi/3$ in a counterclockwise direction are denoted by numbers 2, 3, 4 and 6 with subscripts indicating the positive direction of the axis according to the following correspondence.

Orientations in the cubic group:

x	y	z	xy	$x\bar{y}$	yz	$y\bar{z}$	zx	$z\bar{x}$
[100]	[010]	[001]	[110]	[$\bar{1}$10]	[011]	[0$\bar{1}$1]	[101]	[10$\bar{1}$]

p	q	r	s
[111]	[$\bar{1}\bar{1}$1]	[1$\bar{1}\bar{1}$]	[$\bar{1}$1$\bar{1}$]

Orientations in the hexagonal group:

x	x'	x''	y	y'	y''	z
[100]	[010]	[$\bar{1}\bar{1}$0]	[120]	[$\bar{2}\bar{1}$0]	[1$\bar{1}$0]	[001]

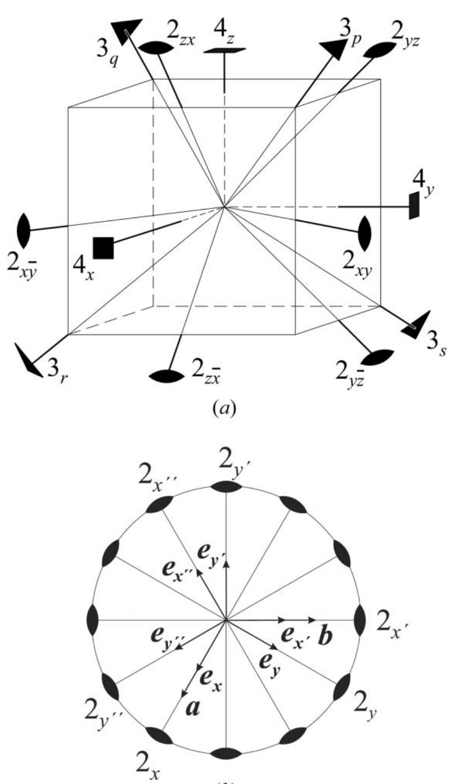

Figure 1
Symbols used for proper rotations

Mirrors are denoted by a common symbol m with the subscript of the twofold axis orthogonal to it. An overbar on the numbers $\bar{3}$, $\bar{4}$ and $\bar{6}$ means a rotoinversion, *i.e.* the combination of rotation with space inversion; the subscript again denotes the positive direction of the axis. The symbols we use throughout for proper rotations are also described visually in Figs. 1(*a*) and 1(*b*) . We use the symbol e for the unit element and i for the space inversion (symbols 1 and $\bar{1}$ are not acceptable in view of the clash with their meaning in Hermann–Mauguin symbols).

Magnetic point groups contain elements combined with the 'magnetic inversion' e' (we avoid the term 'time inversion', which may lead to misinterpretations). We follow the common consensus to distinguish these elements by a prime, so that $g' = ge' = e'g$. Combination of the space and magnetic inversion is denoted by $i' = ie' = e'i$. Again we avoid the use of symbols $1'$ and $\bar{1}'$, which are reserved for Hermann–Mauguin symbols.

Standard orientations: It is necessary and sufficient to choose just one specifically oriented group from each geometric class as a representative of the parent point G in the consideration of ferroic phase transitions. For cubic groups, we use the same orientation as for the cubic group $O_h - m\bar{3}m$. For groups of the tetragonal class and of the hexagonal family, we use the orientation in which the main axis is directed along the vector $\mathbf{e}_z$, one of the auxiliary axes along the vector $\mathbf{e}_x$. We introduce, however, three standard orientations for the monoclinic geometric classes C_{2h}, C_2, C_s, three for the orthorhombic geometric class C_{2v}, and two standard orientations for groups of geometric classes D_{2d}, D_3, C_{3v}, D_{3d} and D_{3h}. There are two reasons for the extension of the choice:

(i) standard orientations of space groups of these geometric classes correspond to several standard orientations of their point groups;

(ii) in systematic tensor calculus, it is suitable to consider equally all groups of the same oriented Laue class (*cf.* §8).

Nonstandard orientations: In consideration of ferroic phase transitions, which constitute the main application of our information scheme, we are interested in the change of tensorial properties when symmetry decreases from that of the parent group G to a low phase symmetry which is one of the conjugate subgroups F_i or a certain normal subgroup H. The parent symmetry can always be chosen as a group in one of the standard orientations and the symmetry of the low phase is always its subgroup. All groups in standard and nonstandard orientations are subgroups of the two specific groups $O_h - m\bar{3}m$ and $D_{6h} - 6_z/m_z m_x m_y$.

Embellished Schoenflies and Hermann–Mauguin symbols: The Schoenflies and Hermann–Mauguin symbols of all specific groups which may appear as the parent or ferroic symmetries in nonmagnetic cases are given in Table 1. The groups are divided into three rows which correspond to subgroups of the group O_h, D_{6h} and to their common subgroups which are all subgroups of the group $D_{2h} = O_h \cap D_{6h}$. The orientation of groups is indicated by directional subscripts which are omitted in cases when misunderstanding is not expected.

The Schoenflies and Hermann–Mauguin symbols for those specific magnetic point groups that appear in this scheme are constructed according to the usual and commonly adopted manner. Schoenflies symbols of groups isomorphic with the proper rotation group G or of nonparamagnetic groups isomorphic with the centrosymmetric group G_h are denoted by $G(H)$ or $G_h(H)$, where H is the halving subgroup of the group G or G_h whose elements are not combined with the magnetic inversion while the elements of the coset to it are combined with the magnetic inversion. Paramagnetic groups are those that contain the magnetic inversion explicitly and they are denoted by primed Schoenflies symbols. In Hermann–Mauguin symbols, the generators that are combined with the magnetic inversion are primed, paramagnetic groups are denoted by the Hermann–Mauguin symbol of the classical group followed by $.1'$. The symbols are embellished by directional subscripts as above.

Spectroscopic symbols: The symbols for elements of the point groups used in the spectroscopic literature are the most frequent among other systems. They are given *e.g.* in tables by Altmann & Herzig (1994) and Bradley & Cracknell (1972). However, the spectroscopic notation is not internally compatible, so that symbols of the same operations differ in different specific groups and even the two books do not have completely identical nomenclature. In addition, some of the symbols clash with Schönflies symbols for the groups. The type of notation described above as the standard one is also used in the literature.

3. Oriented Laue classes of magnetic point groups

The magnetic point groups are subgroups of the group $\mathcal{O}'(3) = \mathcal{O}(3) \otimes E'$, where $E' = \{e, e'\}$ is the magnetic inversion group, e' is the magnetic inversion that changes the sign of each of the magnetic vectors, *i.e.* the magnetic field $\mathbf{H}$, the magnetic induction $\mathbf{B}$ and the magnetization $\mathbf{M}$. Since the group $\mathcal{O}(3)$ itself is a direct product $\mathcal{SO}(3) \otimes I$, where $I = \{e, i\}$ is the space inversion, we can express the whole group $\mathcal{O}'(3)$ as

$$\mathcal{O}'(3) = \mathcal{SO}(3) \otimes E'_o = \mathcal{SO}(3) \cup i\mathcal{SO}(3) \cup e'\mathcal{SO}(3) \cup i'\mathcal{SO}(3),$$

where $E'_o = E' \otimes I = \{e, i, e', i'\}$ is the group of all inversions.

Thus the elements of a magnetic group are of the four types: (i) proper rotations $g \in \mathcal{SO}(3)$, (ii) improper rotations $ig \in i\mathcal{SO}(3)$, (iii) proper magnetic rotations $e'g \in e'\mathcal{SO}(3)$, and (iv) improper magnetic rotations $i'g \in i'\mathcal{SO}(3)$. To each magnetic group (including the classical groups), we can assign a proper rotation group G, which will be obtained if elements ig, $e'g$ and $i'g$ are replaced by proper rotation g. *Vice versa*, each magnetic group can be derived from such a proper rotation group by the method of halving subgroups as has been done in the past in the derivation of both magnetic point and space groups.

Oriented Laue class of magnetic point groups: If a proper rotation group G has a certain orientation, then all magnetic groups derived from it constitute an oriented Laue class of magnetic groups. We shall use only such orientations of parent magnetic groups of ferroic transitions that belong to a Laue class of one of the standard orientations of groups of proper rotations and such orientations of ferroic magnetic groups that belong to oriented Laue classes of groups from Table 1.

Let us briefly recall how the groups of an oriented Laue class are generated by the group of proper rotations G. We apply the method of halving subgroups starting the derivation from groups of proper rotations to emphasize the combination of the three inversions i, e' and i' with cosets to halving or quartering subgroups of these groups. Three cases should be distinguished.

(i) If the group G of proper rotations has no halving subgroup, then only the following magnetic groups can be derived from it: the centrosymmetric group $G_h = G \otimes I$, the group $G_h(G) = G \otimes I'$ and the paramagnetic group $G' = G \otimes E'$, isomorphic with it and the centrosymmetric paramagnetic group $G'_h = G \otimes E'_o$.

Table 1
Schoenflies and Hermann–Mauguin symbols of groups in standard orientations and of their subgroups.

Cubic system			Hexagonal family
$T_h - m\bar{3}$	$O_h - m\bar{3}m$ $O - 432$ $T - 23$	$T_d - \bar{4}3m$	

Tetragonal system			Hexagonal system
$D_{4hz} - 4_z/m_z m_x m_{xy}$	$D_{4hx} - 4_x/m_x m_y m_{yz}$	$D_{4hy} - 4_y/m_y m_z m_{zx}$	$D_{6h} - 6_z/m_z m_x m_y$
$D_{4z} - 4_z 2_x 2_{xy}$	$D_{4x} - 4_x 2_y 2_{yz}$	$D_{4y} - 4_y 2_z 2_{zx}$	$D_6 - 6_z 2_x 2_y$
$C_{4vz} - \underline{4}_z m_x m_{xy}$	$C_{4vx} - \underline{4}_x m_y m_{yz}$	$C_{4vy} - \underline{4}_y m_z m_{zx}$	$C_{6v} - \underline{6}_z m_x m_y$
$\underline{D}_{2dz} - \underline{\bar{4}}_z 2_x m_{xy}$	$\underline{D}_{2dx} - \underline{\bar{4}}_x 2_y m_{yz}$	$\underline{D}_{2dy} - \underline{\bar{4}}_y 2_z m_{zx}$	$\underline{D}_{3h} - \underline{\bar{6}}_z 2_x m_y$
$\widehat{D}_{2dz} - \bar{4}_z m_x 2_{xy}$	$\widehat{D}_{2dx} - \bar{4}_x m_y 2_{yz}$	$\widehat{D}_{2dy} - \bar{4}_y m_z 2_{zx}$	$\widehat{D}_{3h} - \bar{6}_z m_x 2_y$
$C_{4hz} - 4_z/m_z$	$C_{4hx} - 4_x/m_x$	$C_{4hy} - 4_y/m_y$	$C_{6h} - 6_z/m_z$
$C_{4z} - \underline{4}_z$	$C_{4x} - \underline{4}_x$	$C_{4y} - \underline{4}_y$	$C_6 - \underline{6}_z$
$S_{4z} - \bar{4}_z$	$S_{4x} - \bar{4}_x$	$S_{4y} - \bar{4}_y$	$C_{3h} - \bar{6}_z$

Trigonal system

Cubic branch				Hexagonal branch	
$D_{3dp} - \bar{3}_p m_{x\bar{y}}$	$D_{3dq} - \bar{3}_q m_{x\bar{y}}$	$D_{3dr} - \bar{3}_r m_{xy}$	$D_{3ds} - \bar{3}_s m_{xy}$	$D_{3dx} - \bar{3}_z m_x$	$D_{3dy} - \bar{3}_z m_y$
$D_{3p} - 3_p 2_{x\bar{y}}$	$D_{3q} - 3_q 2_{x\bar{y}}$	$D_{3r} - 3_r 2_{xy}$	$D_{3s} - 3_s 2_{xy}$	$D_{3x} - 3_z 2_x$	$D_{3y} - 3_z 2_y$
$C_{3vp} - 3_p m_{x\bar{y}}$	$C_{3vq} - 3_q m_{x\bar{y}}$	$C_{3vr} - 3_r m_{xy}$	$C_{3vs} - 3_s m_{xy}$	$C_{3vx} - 3_z m_x$	$C_{3vy} - 3_z m_y$
$C_{3ip} - \bar{3}_p$	$C_{3iq} - \bar{3}_q$	$C_{3ir} - \bar{3}_r$	$C_{3is} - \bar{3}_s$	$C_{3i} - \bar{3}_z$	
$C_{3p} - 3_p$	$C_{3q} - 3_q$	$C_{3r} - 3_r$	$C_{3s} - 3_s$	$C_3 - 3_z$	

Orthorhombic system

Cubic branch			Common	Hexagonal branch	
$\widehat{D}_{2hz} - m_{x\bar{y}} m_{xy} m_z$	$\widehat{D}_{2hx} - m_{y\bar{z}} m_{yz} m_x$	$\widehat{D}_{2hy} - m_{z\bar{x}} m_{zx} m_y$	$D_{2h} - m_x m_y m_z$	$D_{2h'} - m_{x'} m_{y'} m_z$	$D_{2h''} - m_{x''} m_{y''} m_z$
$\widehat{D}_{2z} - 2_{x\bar{y}} 2_{xy} 2_z$	$\widehat{D}_{2x} - 2_{y\bar{z}} 2_{yz} 2_x$	$\widehat{D}_{2y} - 2_{z\bar{x}} 2_{zx} 2_y$	$D_2 - 2_x 2_y 2_z$	$D_{2'} - 2_{x'} 2_{y'} 2_z$	$D_{2''} - 2_{x''} 2_{y''} 2_z$
$\widehat{C}_{2vz} - m_{x\bar{y}} m_{xy} 2_z$	$\widehat{C}_{2vxy} - m_{x\bar{y}} 2_{xy} m_z$	$\widehat{C}_{2vx\bar{y}} - 2_{x\bar{y}} m_{xy} m_z$	$C_{2vz} - m_x m_y 2_z$	$C_{2vz'} - m_{x'} m_{y'} 2_z$	$C_{2vz''} - m_{x''} m_{y''} 2_z$
$\widehat{C}_{2vx} - m_{y\bar{z}} m_{yz} 2_x$	$\widehat{C}_{2vyz} - m_{y\bar{z}} 2_{yz} m_x$	$\widehat{C}_{2vy\bar{z}} - 2_{y\bar{z}} m_{yz} m_x$	$C_{2vx} - 2_x m_y m_z$	$C_{2vx'} - 2_{x'} m_{y'} m_z$	$C_{2vx''} - 2_{x''} m_{y''} m_z$
$\widehat{C}_{2vy} - m_{z\bar{x}} m_{zx} 2_y$	$\widehat{C}_{2vzx} - m_{z\bar{x}} 2_{zx} m_y$	$\widehat{C}_{2vz\bar{x}} - 2_{z\bar{x}} m_{zx} m_y$	$C_{2vy} - m_x 2_y m_z$	$C_{2vy'} - m_{x'} 2_{y'} m_z$	$C_{2vy''} - m_{x''} 2_{y''} m_z$

Monoclinic system

Cubic branch		Common	Hexagonal branch	
$C_{2hxy} - 2_{xy}/m_{xy}$	$C_{2hx\bar{y}} - 2_{x\bar{y}}/m_{x\bar{y}}$	$C_{2hz} - 2_z/m_z$		
$C_{2hyz} - 2_{yz}/m_{yz}$	$C_{2hy\bar{z}} - 2_{y\bar{z}}/m_{y\bar{z}}$	$C_{2hx} - 2_x/m_x$	$C_{2hx'} - 2_{x'}/m_{x'}$	$C_{2hx''} - 2_{x''}/m_{x''}$
$C_{2hzx} - 2_{zx}/m_{zx}$	$C_{2hz\bar{x}} - 2_{z\bar{x}}/m_{z\bar{x}}$	$C_{2hy} - 2_y/m_y$	$C_{2hy'} - 2_{y'}/m_{y'}$	$C_{2hy''} - 2_{y''}/m_{y''}$
$C_{2xy} - 2_{xy}$	$C_{2x\bar{y}} - 2_{x\bar{y}}$	$C_{2z} - 2_z$		
$C_{2yz} - 2_{yz}$	$C_{2y\bar{z}} - 2_{y\bar{z}}$	$C_{2x} - 2_x$	$C_{2x'} - 2_{x'}$	$C_{2x''} - 2_{x''}$
$C_{2zx} - 2_{zx}$	$C_{2z\bar{x}} - 2_{z\bar{x}}$	$C_{2y} - 2_y$	$C_{2y'} - 2_{y'}$	$C_{2y''} - 2_{y''}$
$C_{sxy} - m_{xy}$	$C_{sx\bar{y}} - m_{x\bar{y}}$	$C_{sz} - m_z$		
$C_{syz} - m_{yz}$	$C_{sy\bar{z}} - m_{y\bar{z}}$	$C_{sx} - m_x$	$C_{sx'} - m_{x'}$	$C_{sx''} - m_{x''}$
$C_{szx} - m_{zx}$	$C_{sz\bar{x}} - m_{z\bar{x}}$	$C_{sy} - m_y$	$C_{sy'} - m_{y'}$	$C_{sy''} - m_{y''}$
		Inversion group $C_i - \bar{1}$ Common to all centrosymmetric groups Identity group $C_1 - 1$ Common to all groups		

(ii) If the group G_1 of proper rotations has exactly one halving subgroup H, so that it can be expressed as $H \cup gH$, we obtain the following set of isomorphic magnetic groups:

(a) $G_1 = H \cup gH$ itself, $G_2 = H \cup igH$, $G_1(H) = H \cup e'gH$ and $G_2(H) = G \cup i'gH$;

(b) the centrosymmetric group $G_h = G \otimes I = H \cup gH \cup iH \cup igH$, three groups: $G_h(G_1) = H \cup gH \cup i'H \cup i'gH$, $G_h(G_2) = H \cup igH \cup e'H \cup i'gH$, $G_h(H_h) = H \cup e'gH \cup iH \cup i'gH$ and two paramagnetic groups $G'_1 = G_1 \otimes E'$, $G'_2 = G_2 \otimes E'$;

(c) the centrosymmetric paramagnetic group $G'_h = G_h \otimes E'_o$.

(iii) If the group G_1 of proper rotations has three halving subgroups H_2, H_3, H_4, it can be expressed as

$$G_1 = H \cup g_2 H \cup g_3 H \cup g_4 H,$$

where $H = H_2 \cap H_3 = H_3 \cap H_4 = H_4 \cap H_2 = H_2 \cap H_3 \cap H_4$ is its quartering subgroup. We introduce groups $H_2 = H \cup g_2H$, $H_3 = H \cup g_3H$, $H_4 = H \cup g_4H$ and groups $K_2 = H \cup ig_2H$, $K_3 = H \cup ig_3H$, $K_4 = H \cup ig_4H$.

(*a*) All magnetic groups of oriented Laue class G_1 isomorphic with the group G_1 can now be arranged into a scheme:

$$\begin{aligned}
G_1 &= H \cup g_2H \cup g_3H \cup g_4H\\
G_1(H_2) &= H \cup g_2H \cup g_3'H \cup g_4'H\\
G_1(H_3) &= H \cup g_2'H \cup g_3H \cup g_4'H\\
G_1(H_4) &= H \cup g_2'H \cup g_3'H \cup g_4H\\
G_2 &= H \cup g_2H \cup ig_3H \cup ig_4H\\
G_2(H_2) &= H \cup g_2H \cup i'g_3H \cup i'g_4H\\
G_2(K_3) &= H \cup g_2'H \cup ig_3H \cup i'g_4H\\
G_2(K_4) &= H \cup g_2'H \cup i'g_3H \cup g_4H\\
G_3 &= H \cup ig_2H \cup g_3H \cup ig_4H\\
G_3(K_2) &= H \cup ig_2H \cup g_3'H \cup ig_4'H\\
G_3(H_3) &= H \cup i'g_2H \cup g_3H \cup i'g_4H\\
G_3(K_4) &= H \cup i'g_2'H \cup g_3'H \cup g_4H\\
G_4 &= H \cup ig_2H \cup ig_3H \cup g_4H\\
G_4(K_2) &= H \cup g_2H \cup i'g_3H \cup i'g_4H\\
G_4(K_3) &= H \cup i'g_2H \cup ig_3H \cup i'g_4H\\
G_4(H_4) &= H \cup i'g_2H \cup i'g_3H \cup g_4H.
\end{aligned}$$

(*b*) We split the groups that are isomorphic with the centrosymmetric group G_{1h} of this class into two categories: (I) groups that do not contain explicitly the magnetic inversion e'; these groups are derived from halving subgroups of the group G_{1h}; (II) groups that are direct products of nonmagnetic groups with E'; these are the groups $G_1' = G_1 \otimes E'$, $G_2' = G_2 \otimes E'$, $G_3' = G_3 \otimes E'$ and $G_4' = G_4 \otimes E'$.

Groups derived by combining cosets of halving subgroups of the group G_{1h} with magnetic inversion can be expressed as

$$\begin{aligned}
G_{1h} &= H \cup g_2H \cup g_3H \cup g_4H \cup iH \cup ig_2H \cup ig_3H \cup ig_4H\\
G_{1h}(H_{2h}) &= H \cup g_2H \cup g_3'H \cup g_4'H \cup iH \cup ig_2H \cup i'g_3H \cup i'g_4H\\
G_{1h}(H_{3h}) &= H \cup g_2'H \cup g_3H \cup g_4'H \cup iH \cup ig_2'H \cup ig_3H \cup ig_4'H\\
G_{1h}(H_{3h}) &= H \cup g_2'H \cup g_3'H \cup g_4H \cup iH \cup i'g_2H \cup i'g_3H \cup ig_4H\\
G_{1h}(G_1) &= H \cup g_2H \cup g_3H \cup g_4H \cup i'H \cup i'g_2H \cup i'g_3H \cup i'g_4H\\
G_{1h}(G_2) &= H \cup g_2H \cup g_3'H \cup g_4'H \cup i'H \cup i'g_2H \cup ig_3H \cup ig_4H\\
G_{1h}(G_3) &= H \cup g_2'H \cup g_3H \cup g_4'H \cup i'H \cup ig_2H \cup i'g_3H \cup ig_4H\\
G_{1h}(G_4) &= H \cup g_2'H \cup g_3'H \cup g_4H \cup i'H \cup ig_2H \cup ig_3H \cup i'g_4H
\end{aligned}$$

(*c*) Finally we obtain exactly one group $G_h' = G \otimes E_o'$.

In these derivations, we use an imitation of the rules for Schoenflies symbols of magnetic point groups, so that subscript h means that $G_h = G \otimes I$, prime means that $G' = G \otimes E'$ and $G_h' = G \otimes E_o'$, while the symbol $G(H) = H \cup g'H$ means that magnetic group which is obtained from the classical group G by combining cosets of its halving subgroup H with magnetic inversion.

In Hermann–Mauguin notation, the symbols of generators are primed if the generator is combined with the magnetic inversion and, if the group is paramagnetic, .1′ is added after the symbol. For the third case, we give, as an example, groups of the oriented Laue class $D_{4z} - 4_z2_x2_{xy}$ in Table 2. The meanings of the symbols in the two columns are connected with representation theory and will be explained later. The groups are divided into the following four categories.

(i) Groups isomorphic with the group of proper rotations G. These can be divided into subsets of magnetic point groups which are derived from the same classical group. Each element of a group of such a subset is then of one of the forms: g, ig, $e'g$, $ie'g$. The choice of isomorphisms is again natural, so that each of such elements is mapped on the element g of the proper rotation group G which generates the oriented Laue class.

(ii) Groups isomorphic with the centrosymmetric group $G_h = G \otimes I$. These are divided into two subsets. (*a*) Magnetic groups derived from the centrosymmetric group. These groups are non-paramagnetic, which means that they do not contain explicitly the magnetic inversion e'. (*b*) Paramagnetic groups, which are direct products of classical groups with the magnetic inversion group $E' = \{e, e'\}$.

(iii) Centrosymmetric paramagnetic group $G_h' = G \otimes I \otimes E'$.

Notice that there are only 11 Laue classes of magnetic crystallographic point groups and hence also of oriented Laue classes of these groups. Each oriented Laue class is generated by a certain proper rotation group and contains only three types of isomorphic groups. A suitable choice of isomorphisms and of labelling the typical variables leads to a situation in which it is sufficient to perform calculation of tensorial covariants and of conversion equations, which is simple but tedious, only for groups of proper rotations and for tensors of even parity with respect to space inversion i and magnetic inversion e'. Analogous tables for other oriented Laue classes including noncrystallographic classes are available on the web pages of the MaThCryst group: http://www.lcm3b.uhp-nancy.fr/mathcryst/.[1]

4. Vector and tensor representations

Quite generally, the term representation is used for various homomorphisms of the group G into some general groups of specific mathematical objects. Point groups themselves are groups of linear operators on the space $V(3)$. Their action on vectors of $V(3)$ induces also their action on various tensor spaces $V^{(u)}(3)$. The action of the group on these spaces is described by matrix representations that assign to each element of the group a certain matrix with reference to a certain basis of the space. The transformation properties of tensors are therefore described by corresponding tensor representations. Magnetic point groups act on tensor spaces $V(3)^{(u)} \times \{1, \tau\}$, where τ is a scalar that changes its sign under

[1] These tables are also available from the IUCr electronic archives (Reference: XO5007). Services for accessing these data are described at the back of the journal.

Table 2
Groups of oriented Laue class $D_{4z} - 4_z 2_x 2_{xy}$ and transformation properties of non-trivial scalars.

		Ireps associated with inversions			Transformation properties of non-trivial scalars		
Class	Group	i	e'	i'	ε	τ	$\varepsilon\tau$
Magnetic point groups, isomorphic with proper rotation group $D_4 - 4_z 2_x 2_{xy}$							
D_4	$4_z 2_x 2_{xy}$	χ_1	χ_1	χ_1	χ_1	χ_1	χ_1
$D_4(C_4)$	$4_z 2'_x 2'_{xy}$	χ_1	χ_2	χ_2	χ_1	χ_2	χ_2
$D_4(D_2)$	$4'_z 2_x 2'_{xy}$	χ_1	χ_3	χ_3	χ_1	χ_3	χ_3
$D_4(\widehat{D}_2)$	$4'_z 2'_x 2_{xy}$	χ_1	χ_4	χ_4	χ_1	χ_4	χ_4
C_{4v}	$4_z m_x m_{xy}$	χ_2	χ_1	χ_2	χ_2	χ_1	χ_2
$C_{4v}(C_4)$	$4_z m'_x m'_{xy}$	χ_2	χ_2	χ_1	χ_2	χ_2	χ_1
$C_{4v}(C_{2v})$	$4'_z m_x m'_{xy}$	χ_2	χ_3	χ_4	χ_2	χ_3	χ_4
$C_{4v}(\widehat{C}_{2v})$	$4'_z m'_x m_{xy}$	χ_2	χ_4	χ_3	χ_2	χ_4	χ_3
D_{2d}	$\bar{4}_z 2_x m_{xy}$	χ_3	χ_1	χ_3	χ_3	χ_1	χ_3
$D_{2d}(S_4)$	$\bar{4}_z 2'_x m'_{xy}$	χ_3	χ_2	χ_4	χ_3	χ_2	χ_4
$D_{2d}(D_2)$	$\bar{4}'_z 2_x m'_{xy}$	χ_3	χ_3	χ_1	χ_3	χ_3	χ_1
$D_{2d}(\widehat{C}_{2v})$	$\bar{4}'_z 2'_x m_{xy}$	χ_3	χ_4	χ_2	χ_3	χ_4	χ_2
$\widehat{D}_{2d}$	$\bar{4}_z m_x 2_{xy}$	χ_4	χ_1	χ_4	χ_4	χ_1	χ_4
$\widehat{D}_{2d}(S_4)$	$\bar{4}_z m'_x 2'_{xy}$	χ_4	χ_2	χ_3	χ_4	χ_2	χ_3
$\widehat{D}_{2d}(C_{2v})$	$\bar{4}'_z m_x 2'_{xy}$	χ_4	χ_3	χ_2	χ_4	χ_3	χ_2
$\widehat{D}_{2d}(\widehat{D}_2)$	$\bar{4}'_z m'_x 2_{xy}$	χ_4	χ_4	χ_1	χ_4	χ_4	χ_1
Nonparamagnetic point groups isomorphic with centrosymmetric group $D_{4h} - 4_z/m_z m_x m_{xy}$							
D_{4h}	$4_z/m_z m_x m_{xy}$	χ_1^-	χ_1^+	χ_1^-	χ_1^-	χ_1^+	χ_1^-
$D_{4h}(C_{4h})$	$4_z/m_z m'_x m'_{xy}$	χ_1^-	χ_2^+	χ_2^-	χ_1^-	χ_2^+	χ_2^-
$D_{4h}(D_{2h})$	$4'_z/m_z m_x m'_{xy}$	χ_1^-	χ_3^+	χ_3^-	χ_1^-	χ_3^+	χ_3^-
$D_{4h}(\widehat{D}_{2h})$	$4'_z/m_z m'_x m_{xy}$	χ_1^-	χ_4^+	χ_4^-	χ_1^-	χ_4^+	χ_4^-
$D_{4h}(D_4)$	$4_z/m'_z m'_x m'_{xy}$	χ_1^-	χ_1^-	χ_1^+	χ_1^-	χ_1^-	χ_1^+
$D_{4h}(C_{4v})$	$4_z/m'_z m_x m_{xy}$	χ_1^-	χ_2^-	χ_2^+	χ_1^-	χ_2^-	χ_2^+
$D_{4h}(D_{2d})$	$4'_z/m'_z m'_x m_{xy}$	χ_1^-	χ_3^-	χ_3^+	χ_1^-	χ_3^-	χ_3^+
$D_{4h}(\widehat{D}_{2d})$	$4'_z/m'_z m_x m'_{xy}$	χ_1^-	χ_4^-	χ_4^+	χ_1^-	χ_4^-	χ_4^+
Noncentrosymmetric paramagnetic groups isomorphic with centrosymmetric group $D_{4h} - 4_z/m_z m_x m_{xy}$							
D'_4	$4_z 2_x 2_{xy}.1'$	χ_{1e}	χ_{1m}	χ_{1m}	χ_{1e}	χ_{1m}	χ_{1m}
C'_{4v}	$4_z m_x m_{xy}.1'$	χ_{2e}	χ_{1m}	χ_{2m}	χ_{2e}	χ_{1m}	χ_{2m}
D'_{2d}	$\bar{4}_z 2_x m_{xy}.1'$	χ_{3e}	χ_{1m}	χ_{3m}	χ_{3e}	χ_{1m}	χ_{3m}
$\widehat{D}_{2d}$	$\bar{4}_z m_x 2_{xy}.1'$	χ_{4e}	χ_{1m}	χ_{4m}	χ_{4e}	χ_{1m}	χ_{4m}
Centrosymmetric paramagnetic group $D'_{4h} - 4_z/m_z m_x m_{xy}.1'$							
D'_{4h}	$4_z/m_z m_x m_{xy}.1'$	χ_{1e}^-	χ_{1m}^+	χ_{1m}^-	χ_{1e}^-	χ_{1m}^+	χ_{1m}^-

the action of magnetic inversion e'. Below we show how matrices of tensor representations are derived from matrices of vector representation.

The vector representation: The point groups are defined as groups of real orthogonal operators $g \in \mathcal{O}(3)$ acting on the three-dimensional vector space $V(3) = V(\mathbf{e}_x, \mathbf{e}_y, \mathbf{e}_z)$. We can say that each point group is its own faithful representation which is called the *vector representation*. The corresponding matrices of the vector representation in the Cartesian (orthonormal) basis $\{\mathbf{e}_x, \mathbf{e}_y, \mathbf{e}_z\}$ will be denoted by $D^{(V)}(g)$. For the purposes of tensor calculus and formulae with summations, we also use an alternative labelling of vectors and their components by numbers as follows:

$$\mathbf{x} = x\mathbf{e}_x + y\mathbf{e}_y + z\mathbf{e}_z = \sum_{i=1}^{3} x_i \mathbf{e}_i,$$

where

$$x = x_1, y = x_2, z = x_3, \quad \mathbf{e}_x = \mathbf{e}_1, \mathbf{e}_y = \mathbf{e}_2, \mathbf{e}_z = \mathbf{e}_3.$$

The action of the point group $G \subseteq \mathcal{O}(3)$ on the space $V(3)$ is defined by

$$g\mathbf{e}_i = \sum_{j=1}^{3} D_{ji}^{(V)}(g)\mathbf{e}_j.$$

If $\mathbf{x} \in V(3)$, then the operator $g \in \mathcal{O}(3)$ sends it to a vector $g\mathbf{x} = \sum_{i=1}^{3} x_i g\mathbf{e}_i = \sum_{i=1}^{3}\sum_{j=1}^{3} D_{ji}^{(V)}(g) x_i \mathbf{e}_j = \sum_{i=1}^{3} x'_i \mathbf{e}_i$, so that the coordinates of the new vector in the old basis are

$$x'_i = (g\mathbf{x})_i = \sum_{j=1}^{3} D_{ij}^{(V)}(g) x_j.$$

This corresponds to the convention by which operators are expressed by square matrices, vectors by column matrices and the action of an operator g on vector $\mathbf{x}$ resulting in vector $\mathbf{x}'$ with coordinates $x'_i = (g\mathbf{x})_i$ is expressed in matrix form by

$$\begin{pmatrix} D_{11}^{(V)}(g) & D_{12}^{(V)}(g) & D_{13}^{(V)}(g) \\ D_{21}^{(V)}(g) & D_{22}^{(V)}(g) & D_{23}^{(V)}(g) \\ D_{31}^{(V)}(g) & D_{32}^{(V)}(g) & D_{33}^{(V)}(g) \end{pmatrix} \begin{pmatrix} x \\ y \\ z \end{pmatrix} = \begin{pmatrix} x' \\ y' \\ z' \end{pmatrix}.$$

The action of the point group $G \subseteq \mathcal{O}(3)$ on the space $V(3)$ also defines the action of this group on spaces of tensors and their components, on polynomials or, more generally, functions of a vector $\mathbf{x} \in V(3)$ or even on polynomials or functions of tensors expressed in terms of their components.

Tensor representations: The vector representation defines tensor representations as follows. We introduce a space $V^n(3) = V^{(u)}$, the basis vectors of which are formally written as

$$\mathbf{e}_{i_1 i_2 \ldots i_n} = \mathbf{e}_{i_1}, \mathbf{e}_{i_2} \ldots, \mathbf{e}_{i_n}.$$

A general element of this space is therefore

$$\mathbf{u} = \sum_{i_1, i_2, \ldots, i_n} u_{i_1 i_2 \ldots i_n} \mathbf{e}_{i_1 i_2 \ldots i_n}.$$

Such an element is called the *tensor of rank n* and the space $V^{(u)}$ is called the *tensor space*. The action of the group G and actually also of the whole orthogonal group $\mathcal{O}(3)$ on this space is defined by the action of its elements on the basis according to

$$\begin{aligned} g\mathbf{e}_{i_1 i_2 \ldots i_n} &= \sum_{j_1, j_2, \ldots j_n} D^{(u)}_{j_1 j_2 \ldots j_n, i_1 i_2 \ldots i_n}(g) \mathbf{e}_{j_1 j_2 \ldots j_n} \\ &= \sum_{j_1, j_2, \ldots j_n} D^{(V)}_{j_1 i_1}(g) D^{(V)}_{j_2 i_2}(g) \ldots D^{(V)}_{j_n i_n}(g) \mathbf{e}_{j_1 j_2 \ldots j_n}, \end{aligned}$$

so that the matrices of the tensor representation are expressed through the matrices of the vector representation as follows:

$$D^{(u)}_{j_1 j_2 \ldots j_n, i_1 i_2 \ldots i_n}(g) = D^{(V)}_{j_1 i_1}(g) D^{(V)}_{j_2 i_2}(g) \ldots D^{(V)}_{j_n i_n}(g).$$

Apart from this, we can define an operation of the symmetric group S_n on this space as the group of permutations of indices $i_1, i_2, \ldots, i_n$. In this way, we can construct tensors of various symmetries with reference to the permutation of indices – the so-called *intrinsic symmetries*. According to a general theorem, tensors of a defined intrinsic symmetry constitute a space that is invariant under the action of the group $\mathcal{O}(3)$ and hence under the point groups $G \subseteq \mathcal{O}(3)$. We define below some tensor spaces of lower orders with symmetrized indices that are used in physics.

The tensor space is just another linear (orthogonalized) space on which the group $\mathcal{O}(3)$ and its subgroups act. Let us denote a tensor of a certain intrinsic symmetry by $\mathbf{A}$, the space of such tensors by $V^{(A)}$ and its basis by $\{\mathbf{e}_i^{(A)}\}_{i \in I(A)}$, where i runs over a certain set of indices $I(A)$. Each index set $I(A)$ is therefore part of the definition of the basis of the tensor space $V^{(A)}$ with reference to which we express the tensor components. There exist standard choices of index sets for tensors of material physics which relate the tensor to a Cartesian coordinate system $(P; \mathbf{e}_x, \mathbf{e}_y, \mathbf{e}_z)$ of the Euclidean space $E(3)$ and hence to an orthonormal (Cartesian) basis $(\mathbf{e}_x, \mathbf{e}_y, \mathbf{e}_z)$ of vector space $V(3)$; corresponding bases $\{\mathbf{e}_i^{(A)}\}_{i \in I(A)}$ will be referred to as *Cartesian bases* of tensor spaces $V^{(A)}$. The general tensor of the space $V^{(A)}$ is expressed as

$$\mathbf{A} = \sum_{i \in I(A)} A_i \mathbf{e}_i^{(A)},$$

where A_i are the Cartesian tensor components. The action of the group $\mathcal{O}(3)$ and of its subgroups G on the space $V^{(A)}$ is given by

$$g\mathbf{A} = \sum_{i \in I(A)} A_i g\mathbf{e}_i^{(A)} = \sum_{i,j \in I(A)} A_i D^{(A)}_{ji}(g) \mathbf{e}_j^{(A)},$$

so that the transformation properties of tensor components are given by

$$(g\mathbf{A})_i = \sum_{i \in I(A)} D^{(A)}_{ij}(g) A_j,$$

where $D^{(A)}_{ij}(g)$ are the matrices of the tensor representation in the basis $\{\mathbf{e}_i^{(A)}\}_{i \in I(A)}$. The calculation of these matrices is actually exactly the procedure we want to avoid.

Why? Well, they are $n \times n$ matrices where n is the dimension of $V^{(A)}$ and the dimensions are unpleasantly high; for example, $n = 6$ for a permittivity or deformation tensor, $n = 18$ for a piezoelectric tensor and $n = 21$ for an elastic stiffness tensor.

How? The answer is given by the theory of irreducible representations which shows how to find the bases in which the action of the group is expressed in the most simplified manner.

5. Irreducible representations

Now we consider the action of a group G on a general linear space $V(n)$ which may be one of the tensor or polynomial spaces. We say that the space $V(n)$ is *reducible* under the action of the group G if the space contains a proper G-invariant subspace $V(m_1)$, otherwise we say that the space is *irreducible*. We say that the space $V(n)$ is *decomposable* under the action of the group G if it splits into a direct sum $V(n) = V(m_1) \oplus V(m_2)$ of G-invariant subspaces $V(m_1)$ and $V(m_2)$, so that each vector $\mathbf{x} \in V(n)$ is uniquely expressible as a sum $\mathbf{x} = \mathbf{x}_1 + \mathbf{x}_2$ of vectors $\mathbf{x}_1 \in V(m_1)$, $\mathbf{x}_2 \in V(m_2)$ and each element $g \in G$ sends a vector $\mathbf{x}_1 \in V(m_1)$ to a vector $g\mathbf{x}_1 \in V(m_1)$ and a vector $\mathbf{x}_2 \in V(m_2)$ to a vector $g\mathbf{x}_2 \in V(m_2)$. If we choose now a basis of the space $V(n)$ in such a manner that m_1 of its vectors $\{\mathbf{e}_1^{(1)}, \ldots, \mathbf{e}_{m_1}^{(1)}\}$ constitute a basis of $V(m_1)$, m_2 of its vectors $\{\mathbf{e}_1^{(2)}, \ldots, \mathbf{e}_{m_2}^{(2)}\}$ constitute a basis of $V(m_2)$, then the matrix form of the action of all elements $g \in G$ will be quasidiagonal:

$$D^{(V)}(g) = \begin{pmatrix} D^{(V_1)}(g) & 0 \\ 0 & D^{(V_2)}(g) \end{pmatrix}.$$

Decomposability is a stronger property than reducibility [*cf.* the action of the point groups on lattices of space groups (Kopský, 2006*c*)]. However, in most applications of group theory to material physics, including our current approach to tensor calculus, reducibility implies decomposability. This is why in textbooks we find only, in general, the concept of reducibility which is handled as if it is decomposability.

The spaces $V(m_1)$, $V(m_2)$ may themselves be further reducible and we can continue the procedure of their further reduction. Eventually we shall arrive at a direct sum $\oplus_{i=1}^{k} V(m_i)$ of k G-invariant irreducible subspaces $V_1 = V(m_1)$,

$V_2 = V(m_2), \ldots, V_k = V(m_k)$ of dimensions m_i, $i = 1, 2, \ldots, k$, with bases $\{\mathbf{e}_1^{(1)}, \ldots, \mathbf{e}_{m_1}^{(1)}\}$, $\{\mathbf{e}_1^{(2)}, \ldots, \mathbf{e}_{m_2}^{(2)}\}$, $\{\mathbf{e}_1^{(k)}, \ldots, \mathbf{e}_{m_k}^{(k)}\}$, in which the matrices of all elements $g \in G$ will have the quasidiagonal form

$$D^{(V)}(g) = \begin{pmatrix} D^{(V_1)}(g) & 0 & \ldots & 0 \\ 0 & D^{(V_2)}(g) & \ldots & 0 \\ \vdots & \vdots & \vdots & \vdots \\ 0 & 0 & \ldots & D^{(V_k)}(g) \end{pmatrix}. \quad (1)$$

Classes of representations and characters: If a group G acts on the space $V(n)$, then the matrices $D^{(V)}(g)$ that represent the action of individual elements $g \in G$ depend on the choice of the basis $\{\mathbf{e}_1, \ldots, \mathbf{e}_n\}$. A transformation $\mathbf{e}'_i = \sum_j^n S_{ji}\mathbf{e}_j$ to another basis $\{\mathbf{e}'_1, \ldots, \mathbf{e}'_n\}$ leads to new matrices $D^{(V)'}(g) = S^{-1}D^{(V)}(g)S$. Two matrix representations related by this similarity transformation are called *equivalent*. Matrix representations of a group G constitute therefore *classes of equivalent representations*. To each class of equivalent representations, we assign a function on the group G by $\chi(g) = \operatorname{Tr} D^{(V)}(g)$, where Tr means the trace of the matrix, *i.e.* the sum of its diagonal elements (another symbol in use is Sp from the German word *Spur*). This function is called the *character* of the representation $D^{(V)}(g)$ and has the following properties.

1. It does not depend on the choice of the basis of $V(n)$ and hence on the particular matrix form of the representation because $\operatorname{Tr} D(g) = \operatorname{Tr} S^{-1}D(g)S$.

2. Characters are functions of conjugacy classes, *i.e.* the elements of the same class K_i have the same character because $\operatorname{Tr} D(fgf^{-1}) = \operatorname{Tr} D(f)D(g)D(f)^{-1} = \operatorname{Tr} D(g)$.

3. The character of the unit element e equals the dimension of the representation: $\chi(e) = \dim V(n) = n$. Indeed, the matrix $D(e)$ contains n times number 1 on the diagonal, so that $\operatorname{Tr} D(e) = n$.

4. If the representation is reducible, then the trace of each matrix $D^{(V)}(g)$ is the sum of traces of the matrices which appear as blocks in the quasidiagonal form, so that $\chi(g) = \sum_{i=1}^k \chi_i(g)$, where $\chi_i(g) = \operatorname{Tr} D^{(V_i)}$.

Characters of irreducible representations: If the group G is finite then the number of equivalence classes of irreducible representations (*ireps*) is finite and equals the number of conjugacy classes in G, *i.e.* the number we denoted by $|K|$. This means that the number of different character functions for irreducible representations is also finite. We give them certain numerical labels $\alpha = 1, 2, \ldots, |K|$ and denote them by $\chi_\alpha(g)$. The label 1 is always reserved for the character $\chi_1(g) = 1$ of the *identity irep*. Irreducible characters have certain marvellous properties.

1. They are mutually orthogonal with respect to averaging over the group G, which means that

$$\frac{1}{|G|}\sum_{g\in G}\chi_\alpha(g)\chi_\beta^*(g) = \delta_{\alpha\beta}, \quad (2)$$

where $\delta_{\alpha\beta}$ is the Kronecker delta, which equals 1 if $\alpha = \beta$, 0 if $\alpha \neq \beta$, and the asterisk denotes complex conjugate.

2. Any representation of G with a character $\chi(g)$ is a direct sum of irreducible representations. The character $\chi(g)$ is the sum

$$\chi(g) = \sum_{\alpha=1}^{|K|} n_\alpha \chi_\alpha(g), \quad (3)$$

in which n_α is the *multiplicity* (or frequency) with which an irep of the class χ_α appears in the representation of the class $\chi(g)$. Using formula (2), we find that the multiplicity equals

$$n_\alpha = \frac{1}{|G|}\sum_{g\in G}\chi(g)\chi_\alpha^*(g). \quad (4)$$

3. Hence the irreducible subspaces $V(m_i)$ can be classified by the ireps of the group G. We give them accordingly labels α, which specify the class of the irep by which the subspace transforms, and labels $a = 1, 2, \ldots, n_\alpha$, which label individual subspaces belonging to the same class of ireps. The whole space is then a direct sum:

$$V(n) = \bigoplus_{\alpha=1}^{|K|}\bigoplus_{a=1}^{n_\alpha} V_{\alpha,a}(d_\alpha) = \bigoplus_{\alpha=1}^{|K|} V_\alpha(n_\alpha d_\alpha), \quad (5)$$

where

$$V_\alpha(n_\alpha d_\alpha) = \bigoplus_{a=1}^{n_\alpha} V_{\alpha,a}(d_\alpha)$$

is the linear envelope of all spaces which transform by the irep of the class χ_α. The subspaces $V_\alpha(n_\alpha d_\alpha)$ are mutually orthogonal, while the subspaces $V_{\alpha a}(d_\alpha)$ can be chosen as orthogonal subspaces but also as non-orthogonal subspaces. Numbers $d_\alpha = \chi_\alpha(e)$ are the dimensions of the irreducible subspaces $V_{\alpha a}(d_\alpha)$.

5.1. The fundamental theorem on representations

To each class $\chi_\alpha(G)$ of ireps of a specific group G, we can choose one certain matrix irep $D^{(\alpha)}: g \longrightarrow D^{(\alpha)}(g)$. Let us consider any space $V(n)$ on which the group G acts as a group of linear operators. If this space splits into G-irreducible subspaces according to relation (5), it is possible to choose the bases $\{\mathbf{e}_{\alpha a,1}, \ldots, \mathbf{e}_{\alpha a,d_\alpha}\}$ of subspaces $V_{\alpha a}$ in such a manner that their vectors transform simultaneously by the same matrix irep $D^{(\alpha)}$, so that

$$g\mathbf{e}_{\alpha a,i} = \sum_{j=1}^{d_\alpha} D_{ji}^{(\alpha)}(g)\mathbf{e}_{\alpha a,j}. \quad (A)$$

If there is only one space $V_\alpha(d_\alpha)$ that transforms by an irep of the class χ_α then the space is uniquely defined and the choice of the basis $\{\mathbf{e}_{\alpha,1}, \ldots, \mathbf{e}_{\alpha,d_\alpha}\}$ which transforms by matrices of $D^{(\alpha)}$ is unique up to a common factor. In other words, all bases that transform by this irep have the form $k\{\mathbf{e}_{\alpha,1}, \ldots, \mathbf{e}_{\alpha,d_\alpha}\} = \{b\mathbf{e}_{\alpha,1}, \ldots, b\mathbf{e}_{\alpha,d_\alpha}\}$, where k is a constant factor; if bases are to be unitary orthonormal, it must be that $|k| = 1$, *i.e.* $k = e^{i\varphi}$; to keep the basis real orthogonal, we have only the choice $k = \pm 1$. If the number of independent subspaces $V_{\alpha a}(d_\alpha)$ is $a = 1, 2, \ldots, n_\alpha > 1$ and their bases are $\{\mathbf{e}_{\alpha a,1}, \ldots, \mathbf{e}_{\alpha a,d_\alpha}\}$, then there exist alternative choices of subspaces $V_{\alpha b}(d_\alpha)$, $b = 1, 2, \ldots, n_\alpha$, with bases $\{\mathbf{e}_{\alpha b,1}, \ldots, \mathbf{e}_{\alpha b,d_\alpha}\}$, related to bases of subspaces $V_{\alpha a}(d_\alpha)$ by

$$\mathbf{e}_{\alpha b,j} = \sum_{a=1}^{n_\alpha} B_{ab}\mathbf{e}_{\alpha a,j}. \tag{i}$$

The counterpart of equations (A) and (i) for components $x_{\alpha a,i}$ of a vector $\mathbf{x} \in V(n)$ in the basis $\{\mathbf{e}_{\alpha a,1}, \ldots, \mathbf{e}_{\alpha a,d_\alpha}\}$ reads

$$(g\mathbf{x})_{\alpha a,i} = \sum_{j=1}^{d_\alpha} D_{ij}^{(\alpha)}(g)x_{\alpha a,j}, \tag{B}$$

$$x_{\alpha b,j} = \sum_{a=1}^{n_\alpha} C_{ba}x_{\alpha a,j}, \tag{ii}$$

where $CB = BC = I$ or $C^{-1} = B$, $B^{-1} = C$. The matrices B and C have to be unitary or orthogonal if we want to keep the bases normalized.

Equations (A), (B) and transformations (i), (ii) constitute the basic relations of the theory of irreducible representations. The bases $\{\mathbf{e}_{\alpha a,1}, \ldots, \mathbf{e}_{\alpha a,d_\alpha}\}$ are further called the $D^{(\alpha)}(G)$ *bases* and the sets of variables $\mathbf{x}_a^{(\alpha)} = (x_{\alpha a,1}, \ldots, x_{\alpha a,d_\alpha})$ are called $D^{(\alpha)}(G)$ *covariants*. The name covariant is of classical origin (Weyl, 1946) and we use it instead of terms like symmetry-adapted basis or form-invariant basis which can be found in the literature. If the irep is one-dimensional, the matrices $D^{(\alpha)}(g)$, $g \in G$, are identical with characters $\chi_\alpha(g)$. In this case, a $\chi_\alpha(G)$ covariant takes the form of one variable $x_{\alpha a}$; such covariants are also called *relative invariants* and, if $\chi_1(G)$ is the identity irep, they are called *invariants*. Covariants are compact mathematical entities; we can define linear combinations of $D^{(\alpha)}(G)$ covariants and hence also the linear independence of $D^{(\alpha)}(G)$ covariants. The advantage of $D^{(\alpha)}(G)$ bases and of $D^{(\alpha)}(G)$ covariants is rather obvious. Instead of handling $n \times n$ matrices which express the action of G on the space $V(n)$, we have to work with minimal possible dimensions of irreducible subspaces which are transformed independently. Of course, if we want to use these advantages, we must develop methods for the calculation of $D^{(\alpha)}(G)$ bases and/or of $D^{(\alpha)}(G)$ covariants. This will be done below with the use of *Clebsch–Gordan products* for tensor spaces.

The contents of this section are a consequence of Schur's Lemma and it is valid only if we consider representations in the field of complex numbers C; we shall use the abbreviation C-irep or just irep. In the consideration of tensor properties, we use representations on real spaces and accordingly we also use the decomposition of these representations into representations which are irreducible over the real field R; sometimes they are called the *physically irreducible representations* or abbreviated as pireps; we shall use the abbreviation R-irep. Some R-ireps do not reduce when the field is extended to C; to those ireps we can apply all the results of the next section; some two-dimensional R-ireps reduce into pairs of complex conjugate C-ireps when the field is extended. The necessary amendment of consequences is simple and we shall handle it in one standard manner later under the heading *The standard transformations* (§6.1).

Remark. In spectroscopy, the consequence of the distinction between R-reducibility and C-reducibility is known as the *Kramers degeneracy*. In its general form, the relationship between R-ireps and C-ireps may be quite complicated. In our cases, we are handling the simplest possible situation.

6. Typical bases and typical covariants

Yet again no unique and generally accepted symbolism of classes of ireps of the point groups exists. The most commonly used spectroscopic notation for classes of ireps uses letters A and B for one-dimensional ireps, E for two-dimensional ireps (left superscripts ^1E and ^2E are used for complex conjugate one-dimensional ireps of groups C_n, $n \geq 3$ and of the group T), letter T is used for three-dimensional ireps of cubic groups [letters F, H and I are used for the four-, five- and six-dimensional ireps which appear either as ireps of the icosahedral group or as double-valued ireps of the cubic and icosahedral group; *cf.* Altmann & Herzig (1994) or Bradley & Cracknell (1972)]. The letters, if used more than once, are distinguished either by numerical subscripts or by primes and double primes. Parities with reference to space inversion i are denoted by subscripts g (German *gerade* = even) and u (German *ungerade* = odd).

Symbols Γ_α with numerical labels α carry even less information. Number $\alpha = 1$ is reserved for the identity irep and ireps of higher dimensions have, as a rule, a higher-valued label. Symbols χ_α are used to denote characters of ireps and superscripts $+$ and $-$ denote the even and odd parities with respect to space inversion. Neither of these symbolisms is sufficient for our purposes. The use of characters is limited to the calculation of *selection rules* or to the numbers of tensor components that transform by various ireps.

To facilitate the work with tensorial bases, we developed the method of typical variables and covariants which proved also to be useful for recording other relations (see paper 2).

Explicit irreducible representations and typical variables: For the purposes of tabulation, it is suitable to introduce rather abstract carrier spaces, bases and variables. The idea is very old and stems from the theory of invariants where an analogous approach is known as the symbolic method (Weitzenböck, 1923). For a given group G, we introduce the *typical carrier space* $V_o = \oplus_{\alpha=1}^{|K|} V_\alpha$ which contains exactly once a carrier space V_α for each class $\chi_\alpha(G)$ of ireps. In each class $\chi_\alpha(G)$, we choose a certain standard matrix irep $D^{(\alpha)}(G)$ of the group G. To this irep there corresponds a basis $\{\mathbf{e}_{\alpha,1}, \ldots, \mathbf{e}_{\alpha,d_\alpha}\}$ called the *typical* $D^{(\alpha)}$ *basis* and a set of variables $\mathbf{x}^{(\alpha)} = (x_{\alpha,1}, \ldots, x_{\alpha,d_\alpha})$, called the *typical variables*. The whole set $\mathbf{x}^{(\alpha)}$ is called the typical $D^{(\alpha)}(G)$ covariant or the typical $\chi_\alpha(G)$ covariant. The concept has been revived together with the term covariant by this author (Kopský, 1976*a*,*b*) for the purposes of suitable recording and handling of transformation properties of tensors and of polynomials. Consequently, the typical variables have been standardized compared to their original labelling; in tables they appear as *standard typical variables*.

The standard typical variables: There remains a certain freedom in the choice of matrix ireps and of their labelling. We developed a special notation for our purposes which is called here the *standard notation*. One of the advantages of this notation is the transparency of subduction relations which correlate the typical variables (and consequently all variables) for a group with variables for its subgroups. The scheme actually includes all finite groups and is extremely convenient for consideration of transformation properties of tensors. First we shall describe the choice of the standard typical variables for groups of proper rotations.

Groups of proper rotations: The standard typical variables for real one-dimensional ireps are denoted by sans-serif letters x_α with numerical subscripts $\alpha = 1, 2, 3, 4$. The index 1 is reserved for that variable which transforms by the identity irep $\chi_1(G)$ so that x_1 is the typical invariant for any group G of proper rotations. Other variables x_α are called the typical relative invariants or the typical $\chi_\alpha(G)$ covariants because the actual variables transforming in the same way are usually called *relative invariants*.

The proper rotation groups D_2 $(2_x 2_y 2_z)$, D_{4z} $(4_z 2_x 2_{xy})$ and D_6 $(6_z 2_x 2_y)$ have four one-dimensional ireps and the labels are chosen so that the subscript 2 corresponds to an irep with kernel C_{2z} (2_z), C_{4z} (4_z) and C_6 (6_z), respectively, while subscript 3 corresponds to ireps with kernels C_{2x} (2_x), D_2 $(2_x 2_y 2_z)$ and D_{3x} $(3_z 2_x)$, subscript 4 to ireps with kernels C_{2y} (2_y), $\hat{D}_2$ $(2_{xy} 2_{x\bar{y}} 2_z)$ and D_{3y} $(3_z 2_y)$. In other words, index 2 indicates that the variable x_2 does not change sign under rotations about the principal axis, index 3 indicates that the variable x_3 does not change sign under the twofold rotations about axes conjugate with 2_x and index 4 indicates that the variable x_4 does not change sign under the action of the other set of conjugate axes. This rule is extended to noncrystallographic proper rotation groups D_n $(n_z 2_{x_1} 2_{x_2})$ with even n.

The proper rotation groups D_{3x} $(3_z 2_x)$, D_{3y} $(3_z 2_y)$ and O (432) have two real one-dimensional ireps and the subscript 2 is used for the non-trivial irep. Hence x_2 is that variable which does not change sign under rotations about the principal axis and changes sign under rotations about the auxiliary axes [in the case of group O (432) it does not change under the elements of the subgroup T (23) and changes sign under the action of elements from the coset of $4_z T$]. Again, the same holds for non-crystallographic proper rotation groups D_n $(n_z 2_x)$ with odd n.

The subgroups C_{2z} (2_z), C_{4z} (4_z) and C_6 (6_z) have two one-dimensional ireps and the non-trivial irep is assigned the subscript 3. Accordingly, the subduction from the respective dihedral groups sends the variables x_1 and x_2 into x_1, the variables x_3 and x_4 into x_3.

The groups D_n and C_n with $n \geq 3$ have two-dimensional real ireps. These ireps are irreducible over the real field and for groups D_n also in the complex field. For the groups C_n, they are reducible in the complex field into a pair of conjugate complex ireps. The variables (x_1, y_1) which appear in all these groups have the meaning of the components of an ordinary vector in the (xy) plane. The variables (x_2, y_2) which appear in groups D_6 and C_6 (actually they appear already in the noncrystallographic groups D_5 and C_5) transform under rotation by an angle φ about the z axis like components of an ordinary vector under rotation by 2φ about the z axis. Analogously, variables (x_n, y_n), $n \geq 3$, which appear in noncrystallographic groups with a higher order of the principal axis, transform under the rotation by an angle φ about z-axis-like components of an ordinary vector under rotation by $n\varphi$ about the z axis. The index n of these variables has an informative value; it is equal to the lowest-rank tensor, the components of which transform like these variables.

Two-dimensional real ireps appear also for groups T (23) and O (432), where variables are denoted by (x_3, y_3). This irep is irreducible over the complex field for the group O (432) and reducible into a pair of conjugate complex ireps in the group T (23).

The reduction of two-dimensional ireps is considered below on a unified basis for all cases in §6.1 *Standard transformations*, where complex variables are introduced to complete the scheme and the consequences of the violation of conditions for Schur's Lemma are explained.

Three-dimensional ireps appear for groups T (23) and O (432), where variables are denoted by (x_1, y_1, z_1). These variables transform like the components of a vector in the space $V(3)$. To the second three-dimensional irep of the group O (432), we assign variables (x_2, y_2, z_2) which transform like the product $\mathsf{x}_2(x_1, y_1, z_1)$ (see also the Clebsch–Gordan product tables which are very illustrative for exploring various relations between transformation properties of standard typical variables) or like the components of an ordinary vector under the action of the group T_d $(\bar{4}3m)$.

Now we shall describe the rules for specification of ireps and standard typical variables for groups of the same oriented Laue class.

Groups which are isomorphic with a proper rotation group G: The standard typical variables for a group isomorphic with G are denoted in the same manner as for the group G. These groups contain elements $g \in G$ in combination with inversions i, e' and i'. We define the transformation properties of standard typical variables by the rule that each of the variables transforms in the same manner under elements ig, $e'g$ or $i'g$ as under the action of g as defined for the group G.

Specification of ireps and standard typical variables for groups of the tetragonal system are given in Table 3. Complete tables for crystallographic Laue classes are presented in the paper by Kopský (2001) and in the software *GI*★*KoBo-1* (Kopský & Boček, 2003) where the correspondence to spectroscopic symbols is also given.

Nonparamagnetic groups, isomorphic with a centrosymmetric group: A centrosymmetric group $G_h = G \otimes I = G \cup iG$ contains all elements $g \in G$ and of the coset $ig = gi \in iG = Gi$. The number of conjugacy classes is doubled compared to the conjugacy classes of G and hence also the number of ireps and variables is doubled. Even and odd ireps are distinguished by superscripts + and −, respectively; these superscripts indicate the parity of the variable

Table 3
Specification of irreducible representations for tetragonal groups.

Groups of oriented Laue class $C_{4hz} - 4_z/m_z$		
$C_{4z} - 4_z$	4_z	
$S_{4z} - \bar{4}_z$	$\bar{4}_z$	
$\chi_1(\mathsf{X}_1)$	1	
$\chi_3(\mathsf{X}_3)$	−1	
$D^{(1)}(x_1, y_1)$	$\begin{pmatrix} 0 & -1 \\ 1 & 0 \end{pmatrix}$	
Groups of oriented Laue class $D_{4hz} - 4_z/m_z m_x m_{xy}$		
$D_{4z} - 4_z 2_x 2_{xy}$	4_z	2_x
$C_{4vz} - 4_z m_x m_{xy}$	4_z	m_x
$D_{2dz} - \bar{4}_z 2_x m_{xy}$	$\bar{4}_z$	2_x
$\widehat{D}_{2dz} - \bar{4}_z m_x 2_{xy}$	$\bar{4}_z$	m_x
$\chi_1(\mathsf{X}_1)$	1	1
$\chi_2(\mathsf{X}_2)$	1	−1
$\chi_3(\mathsf{X}_3)$	−1	1
$\chi_4(\mathsf{X}_4)$	−1	−1
$D^{(1)}(x_1, y_1)$	$\begin{pmatrix} 0 & -1 \\ 1 & 0 \end{pmatrix}$	$\begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}$

under the action of the space inversion i; variables with the superscript $+$ do not change sign, variables with the superscript $-$ change sign under the action of i. Each variable x^+ then transforms in the same way under the action of both elements $g \in G$ and $ig \in iG$ as the variable x transforms under the element $g \in G$, while the variable x^- transforms under an element $g \in G$ in the same way as x and under the action of $ig \in iG$ it transforms in the same way as x under the action of $g \in G$ with an additional change of the sign.

Nonparamagnetic groups, isomorphic with G_h, contain some elements of G_h combined with the magnetic inversion e'. These are the elements of the coset to halving subgroups of G_h. If we denote now by g elements of G_h, then these cosets contain elements $h' = e'h = he'$. We define the transformation properties of standard typical variables under the action of these groups so that x^+ as well as x^- transform in the same manner under the element h' as it transforms under the element h.

Paramagnetic noncentrosymmetric groups: These groups are of the form of direct product $G' = G \otimes E' = G \cup e'G$, where $G = H \cup igH$ is a classical group (including G itself). The number of conjugacy classes as well as ireps is doubled. We distinguish variables by parity subscripts e and m where e indicates positive, m negative parity. Hence a variable x_e transforms in the same way under the action of elements g and $e'g$, as x transforms under the action of g, while the variable x_m transforms in the same way under the action of g but changes in addition its sign under the action of $e'g$.

The centrosymmetric paramagnetic group: There is one such group in each oriented Laue class and it has the form $G'_h = G \otimes E'_o = G \cup iG \cup e'G \cup i'G$. The number of conjugacy classes, of ireps and of typical standard variables is four times that for the group G and we distinguish the variables by both parity labels. Thus we have four variables: $x_e^+, x_e^-, x_m^+, x_m^-$, which transform in the same way under elements $g \in G$ but in addition change sign according to their parities, so that superscript $-$ indicates an additional change of sign under the action of i', subscript m an additional change of sign under the action of e'. Thus variables x_e^- and x_m^+ change sign under the action of i'.

Remark. Not only is the described choice of matrix ireps and of typical variables the most natural but it is also the choice which enables us to use Opechowski's magic relations. In the second column of Table 2 are listed one-dimensional ireps of groups associated with inversion i, e', i'. These are those ireps of magnetic point groups in the table whose kernels are the halving subgroups which do not contain the respective inversions, while elements of their cosets are combined with these inversions. The full implications are explained in §8.

6.1. The standard transformations

The action of a rotation by φ around the z axis, denoted as an operator $g(\varphi)$, is expressed in the Cartesian basis $(\mathbf{e}_x, \mathbf{e}_y, \mathbf{e}_z)$ by the equations

$$\begin{aligned} g(\varphi)\mathbf{e}_x &= \mathbf{e}_x \cos\varphi + \mathbf{e}_y \sin\varphi, \\ g(\varphi)\mathbf{e}_y &= -\mathbf{e}_x \sin\varphi + \mathbf{e}_y \cos\varphi, \\ g(\varphi)\mathbf{e}_z &= \mathbf{e}_z, \end{aligned}$$

to which there corresponds a matrix

$$D_R^{(1)}[g(\varphi)] = \begin{pmatrix} \cos\varphi & -\sin\varphi & 0 \\ \sin\varphi & \cos\varphi & 0 \\ 0 & 0 & 1 \end{pmatrix}$$

of a real vector representation $D_R^{(1)}$. These vectors transform under the action of twofold rotation 2_x as

$$2_x\mathbf{e}_x = \mathbf{e}_x, \quad 2_x\mathbf{e}_y = -\mathbf{e}_y, \quad 2_x\mathbf{e}_z = -\mathbf{e}_z,$$

which is expressed by the matrix

$$D_R^{(1)}(2_x) = \begin{pmatrix} 1 & 0 & 0 \\ 0 & -1 & 0 \\ 0 & 0 & -1 \end{pmatrix}.$$

We introduce standard typical vectors $(\mathbf{e}_{nx}, \mathbf{e}_{ny})$ in the $x_n y_n$ plane which transform by definition under the action of $g(\varphi)$ and 2_x according to equations

$$\begin{aligned} g(\varphi)\mathbf{e}_{nx} &= \mathbf{e}_{nx} \cos n\varphi + \mathbf{e}_{ny} \sin n\varphi, \\ g(\varphi)\mathbf{e}_{ny} &= -\mathbf{e}_{nx} \sin n\varphi + \mathbf{e}_{ny} \cos n\varphi, \\ 2_x\mathbf{e}_{nx} &= \mathbf{e}_{nx}, \quad 2_x\mathbf{e}_{ny} = -\mathbf{e}_{ny}. \end{aligned}$$

To these transformations there correspond the matrices

$$D_R^{(n)}[g(\varphi)] = \begin{pmatrix} \cos n\varphi & -\sin n\varphi \\ \sin n\varphi & \cos n\varphi \end{pmatrix} \quad \text{and} \quad D_R^{(n)}(2_x) = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}$$

of a real vector representation $D_R^{(n)}$.

We introduce a standard transformation to complex vectors and variables:

$$\mathbf{e}_{n\xi} = \frac{1}{\sqrt{2}}(\mathbf{e}_{nx} - i\mathbf{e}_{ny}), \quad \mathbf{e}_{n\eta} = \frac{1}{\sqrt{2}}(\mathbf{e}_{nx} + i\mathbf{e}_{ny}),$$
$$\xi_n = \frac{1}{\sqrt{2}}(x_n + iy_n), \quad \eta_n = \frac{1}{\sqrt{2}}(x_n - iy_n).$$

The reciprocal transformation then reads

$$\mathbf{e}_{nx} = \frac{1}{2^{1/2}}(\mathbf{e}_{n\xi} + \mathbf{e}_{n\eta}), \quad \mathbf{e}_{ny} = \frac{i}{2^{1/2}}(\mathbf{e}_{n\xi} - i\mathbf{e}_{n\eta}),$$
$$x_n = \frac{1}{2^{1/2}}(\xi_n + \eta_n), \quad y_n = \frac{i}{2^{1/2}}(\eta_n - \xi_n).$$

Vectors are then expressed in the two bases as

$$\mathbf{x}_n = x_n\mathbf{e}_{nx} + y_n\mathbf{e}_{ny} = \xi_n\mathbf{e}_{n\xi} + \eta_n\mathbf{e}_{n\eta},$$

and the transformation properties of complex vectors and bases are expressed by

$$g(\varphi)\mathbf{e}_{n\xi} = \mathrm{e}^{in\varphi}\mathbf{e}_{n\xi}, \quad g(\varphi)\mathbf{e}_{n\eta} = \mathrm{e}^{-i\varphi}\mathbf{e}_{n\eta},$$
$$2_x\mathbf{e}_{n\xi} = \mathbf{e}_{n\eta}, \quad 2_x\mathbf{e}_{n\eta} = \mathbf{e}_{n\xi},$$

so that the rotations are expressed by matrices

$$D_C^{(n)}[g(\varphi)] = \begin{pmatrix} \mathrm{e}^{in\varphi} & 0 \\ 0 & \mathrm{e}^{-in\varphi} \end{pmatrix} \quad \text{and} \quad D_C^{(n)}(2_x) = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}.$$

The real pair of variables (x_n, y_n) is transformed to a complex pair (ξ_n, η_n) and the real matrix irep $D_R^{(n)}$ to an equivalent complex matrix irep $D_C^{(n)}$. Both ireps are irreducible for groups D_n, $n \geq 3$ because the twofold rotation 2_x swaps the vectors $\mathbf{e}_{n\xi}$, $\mathbf{e}_{n\eta}$ as well as the variables ξ_n, η_n.

Matrices $D_C^{(n)}[g(\varphi)]$ are, however, quasidiagonal (in fact they are diagonal) and correspond to a pair of one-dimensional complex conjugate ireps. Two-dimensional representations of uniaxial groups and of groups T (23) and T_h ($m\bar{3}$) are therefore irreducible over the real field but they split into a pair of one-dimensional complex conjugate ireps in the complex field. As a consequence, the pair of variables (x_n, y_n) transforms under these groups in the same way as the pair $(y_n, -x_n)$.

7. The Clebsch–Gordan products

If the basis vectors $(\mathbf{e}_{\alpha,1}, \mathbf{e}_{\alpha,2}, \ldots, \mathbf{e}_{\alpha,d_\alpha})$ of the carrier space V_α for an irep $D^{(\alpha)}(G)$ are combined with the basis vectors $(\mathbf{e}_{\beta,1}, \mathbf{e}_{\beta,2}, \ldots, \mathbf{e}_{\beta,d_\beta})$ of the carrier space V_β for an irep $D^{(\beta)}(G)$, we obtain a set of $d_\alpha d_\beta$ basis vectors $(\mathbf{e}_{\alpha,i}\mathbf{e}_{\beta,j})$ of the carrier space $V_\alpha \otimes V_\beta$ which is called the *direct* or *tensor product* of spaces V_α and V_β.

The latter space is generally reducible and spaces of the type V_γ appear in the reduction with certain multiplicities $m_{(\alpha,\beta|\gamma)} = (1/|G|)\sum_{g\in G}\chi_\alpha(g)\chi_\beta(g)\chi_\gamma^*(g)$. If the two spaces in the product belong to the same irep $D^{(\alpha)}(G)$, then the product space $V_\alpha \otimes V_\alpha$ splits into the space of symmetric and antisymmetric combinations with bases

$$\frac{1}{2^{1/2}}(\mathbf{e}_{\alpha,i_\alpha}\mathbf{e}_{\alpha,j_\alpha} + \mathbf{e}_{\alpha,j_\alpha}\mathbf{e}_{\alpha,i_\alpha}) \quad \text{and} \quad \frac{1}{2^{1/2}}(\mathbf{e}_{\alpha,i_\alpha}\mathbf{e}_{\alpha,j_\alpha} - \mathbf{e}_{\alpha,j_\alpha}\mathbf{e}_{\alpha,i_\alpha}).$$

The spaces are usually denoted as $[V_\alpha]^2$ for the symmetric case and $\{V_\alpha\}^2$ for the antisymmetric case and both spaces are invariant under the action of G and are generally reducible. The multiplicities then split into the sum of multiplicities for the symmetric and antisymmetric parts: $m_{(\alpha,\alpha|\gamma)} = m_{[\alpha,\alpha|\gamma]} + m_{\{\alpha,\alpha|\gamma\}}$. Multiplicities are sometimes called the Clebsch–Gordan or Wigner coefficients and the products of matrices are called the Kronecker products (Bradley & Cracknell, 1972).

The tables of Kronecker products facilitate the calculation of selection rules and they are widely used in spectroscopy. They can also be used to calculate the numbers of independent tensor components and hence to find how many new independent parameters appear in a tensor at a phase transition or the numbers of components in which two domain states differ. The tables of Clebsch–Gordan products, described in this section, represent an explicit counterpart of the Kronecker product tables and they facilitate the calculation of explicit tensor components.

Clebsch–Gordan products: Our calculations of tensorial covariants are based on the method of Clebsch–Gordan products in typical variables. The method stems originally from the theory of quantum momentum. Irreducible representations of the orthogonal group $\mathcal{O}(3)$ are labelled by the quantum number j of the total momentum and the wavefunctions ψ_{jm} form irreducible spaces of dimension $2j+1$ with $m = -j, \ldots, j-1, j$, where m defines the projection of the momentum on a chosen axis, usually the z axis. In a system of two particles in a spherical field, the total wavefunction Ψ_{JM} is expressed as

$$\Psi_{JM} = \sum_{m_1+m_2=M}(j_1m_1j_2m_2|JM)\psi_{j_1m_1}\psi_{j_2m_2}, \qquad \text{(iii)}$$

where $(j_1m_1j_2m_2|JM)$ are the so-called Clebsch–Gordan coefficients, also called the coefficients of vector addition.

Quite analogously, we can introduce Clebsch–Gordan coefficients for the multiplication of irreducible representations of any group G. The direct product $V_\alpha \otimes V_\beta$ of two typical irreducible spaces splits according to the fundamental theorem into irreducible subspaces $V_{\gamma m}$, where $m = 1, 2, \ldots, m_{(\alpha,\beta|\gamma)} = \frac{1}{|G|}\sum_{g\in G}\chi_\alpha(g)\chi_\beta(g)\chi_\gamma^*(g)$. The generalized Clebsch–Gordan formula reads

$$\mathbf{E}_{\gamma k}^{(m)} = \sum_{i=1}^{d_\alpha}\sum_{j=1}^{d_\beta}(\alpha i\beta j|\gamma k)^{(m)}\mathbf{e}_{\alpha,i}\mathbf{e}_{\beta,j}. \qquad \text{(iv)}$$

The label m does not appear in the classical formula (iii) because multiplicities are in this case always $m(j_1, j_2|J) = 1$. We can also rewrite the latter formula in terms of the standard variables:

$$X_{\gamma k}^{(m)} = \sum_{i=1}^{d_\alpha}\sum_{j=1}^{d_\beta}(\alpha i\beta j|\gamma k)^{(m)*}x_{\alpha i}x_{\beta j}, \qquad \text{(v)}$$

and in the case $\alpha = \beta$ we also have to distinguish the symmetrized and antisymmetrized cases. Clebsch–Gordan coefficients $(\alpha i\beta j|\gamma k)^{(m)}$ for the crystal point groups were calculated by Koster *et al.* (1963). They are important in quantum-mechanical calculations when orthonormality of wavefunctions is required.

Our aim is to find transformation properties of tensors and we can disregard the normalization conditions. For calculations of this type, tables of Clebsch–Gordan products are more convenient. Without writing formulas, we define Clebsch–Gordan products for the set of ireps of the group G as those $D^{(\gamma)}(G)$ covariants whose components are bilinear combinations of components of a typical $D^{(\alpha)}(G)$ covariant $(x_{\alpha 1}, \ldots, x_{\alpha d_\alpha})$ and $D^{(\beta)}(G)$ covariant $(x_{\beta 1}, \ldots, x_{\beta d_\beta})$. The number of such independent covariants is given by Kronecker products but their calculation for the crystal point groups is relatively easy. They are collected in tables where the heading of each table lists the typical $D^{(\gamma)}(G)$ covariants and in the column headed by such a covariant are given bilinear combinations of typical variables which transform in the same way as the variables $(x_{\gamma 1}, \ldots, x_{\gamma d_\gamma})$. This is actually just another way to record the full set of relations (v); to get the Clebsch–Gordan coefficients from tables of Clebsch–Gordan products it is sufficient to perform the normalization.

It is necessary to realize that the variables in the tables are just the representatives of actual variables. In the calculation of the tensor product of any two spaces V_1 and V_2, we first find the linear combinations of vector components in the two spaces which transform like the typical variables. In this procedure, several actual covariants may appear corresponding to some ireps. The tables give the prescription how to form their bilinear combinations of the desired transformation properties. Such tables were published and their use described a quarter of century ago (Kopský, 1976*a*,*b*, 1977). Revised definition of standards of ireps and symbols of typical variables is given in Appendix *C* for crystallographic groups of proper rotations and the respective tables of Clebsch–Gordan products are given in Appendix *D* of the monograph by Kopský (2001). In Table 4, we illustrate the form of these tables using the example of groups C_{4z} (4_z) and D_{4z} ($4_z2_x2_{xy}$).

Trivial Clebsch–Gordan products $\mathsf{x}_1(x_{\alpha 1}, \ldots, x_{\alpha d_\alpha})$ and $(x_{\alpha 1}, \ldots, x_{\alpha d_\alpha})\mathsf{x}_1$ are not explicitly written down in the tables; it is clear that they transform like $(x_{\alpha 1}, \ldots, x_{\alpha d_\alpha})$. The antisymmetric expressions like $x_1y_1 - y_1x_1$ express formally all possible bilinear combinations $x_1^{(a)}y_1^{(b)} - y_1^{(a)}x_1^{(b)}$, where a, b label various spaces and such combinations vanish when $a = b$. To such a product as $\mathsf{x}_3\mathsf{x}_4$ there naturally corresponds the product $\mathsf{x}_4\mathsf{x}_3$ which is not given in the tables. If replaced by actual variables, we have to distinguish the symmetric $(\mathsf{x}_3^{(a)}\mathsf{x}_4^{(b)} + \mathsf{x}_4^{(a)}\mathsf{x}_3^{(b)})$ and antisymmetric $(\mathsf{x}_3^{(a)}\mathsf{x}_4^{(b)} - \mathsf{x}_4^{(a)}\mathsf{x}_3^{(b)})$ combinations which both transform like the product $\mathsf{x}_3\mathsf{x}_4$. Analogous considerations hold in the case of products of the type $\mathsf{x}_\alpha(x_1, y_1, z_1)$ to which there correspond products $(x_1, y_1, z_1)\mathsf{x}_\alpha$. Quite generally, for a certain Clebsch–Gordan product which combines variables of two ireps of different classes in a certain order there exists a Clebsch–Gordan product in which the order is reversed. If the typical variables are then replaced by actual ones, we should create the symmetric and antisymmetric combinations.

The tables are given in terms of variables which correspond to the relation (v). Analogous tables can be written for basis vectors. The presentation in terms of variables (components of vectors) is more convenient for our proceeding further. The two tables apply to all magnetic point groups which are isomorphic to the two groups. Clebsch–Gordan tables for a centrosymmetric group and its isomorphs are easily deduced from these tables. Instead of each variable x, we have two variables: x^+ and x^- and their bilinear products obey the parity rules. The same concerns Clebsch–Gordan tables for paramagnetic groups with variables x_e and x_m and for the centrosymmetric paramagnetic group with variables x_e^+, x_e^-, x_m^+, x_m^-.

Table 4
Clebsch–Gordan products for tetragonal groups.

Group $C_4 - 4_z$

x_1	x_3	(x_1, y_1)
x_3^2		
$x_1^2 + y_1^2$	$x_1^2 - y_1^2$	$\mathsf{x}_3(x_1, -y_1)$
$x_1y_1 - y_1x_1$	$x_1y_1 + y_1x_1$	

In view of the reducibility of the irep $D_R^{(1)}(C_{4z})$ in complex field, there exist also $D_R^{(1)}(C_{4z})$ covariants $(y_1, -x_1)$ and $\mathsf{x}_3(y_1, x_1)$.

Group $D_4 - 4_z2_x2_{xy}$

x_1	x_2	x_3	x_4	(x_1, y_1)
$\mathsf{x}_2^2\ \mathsf{x}_3^2\ \mathsf{x}_4^2$	$\mathsf{x}_3\mathsf{x}_4$	$\mathsf{x}_2\mathsf{x}_4$	$\mathsf{x}_2\mathsf{x}_3$	$\mathsf{x}_2(y_1, -x_1)$
$x_1^2 + y_1^2$	$x_1y_1 - y_1x_1$	$x_1^2 - y_1^2$	$x_1y_1 + y_1x_1$	$\mathsf{x}_3(x_1, -y_1)$
				$\mathsf{x}_4(y_1, x_1)$

8. Calculation of tensorial covariants

We shall consider now the space $V^{(A)}$ of a certain tensor $\mathbf{A}$ under the action of a point group G. Using the fundamental theorem on representations, we can write the tensor in the form

$$\mathbf{A} = \sum_{i \in I(A)} A_i \mathbf{e}_i^{(A)} = \sum_{\alpha=1}^{K} \sum_{a=1}^{n_\alpha} \sum_{i=1}^{d_\alpha} A_{\alpha a,i} \mathbf{e}_{\alpha a,i},$$

where the first sum is the expression of the tensor in a Cartesian reference basis $\{\mathbf{e}_i^{(A)}\}_{i \in I(A)}$ while in the second expression we express the tensor in $D^{(\alpha)}(G)$ bases $\mathbf{e}_{\alpha a,i}$, so that the coefficients form the $D^{(\alpha)}(G)$ covariants $\mathbf{A}_a^{(\alpha)} = (A_{\alpha a,1}, A_{\alpha a,2}, \ldots, A_{\alpha a,d_\alpha})$. The number of ireps equals K which is also the number of classes of conjugate elements in G, $n_\alpha = (1/|G|) \sum_{g \in G} \chi^{(A)}(g)\chi_\alpha^*(g)$ is the multiplicity with which the irep of the class $\chi_\alpha(G)$ appears in the tensor representation $D^{(A)}(G)$ and $d_\alpha = \chi_\alpha(e)$ is the dimension of this irep. The dimension of the tensor space satisfies the relation $\dim V^{(A)} = \sum_\alpha n_\alpha d_\alpha$.

The expression for the tensor $\mathbf{A}$ in $D^{(\alpha)}(G)$ bases is called the *decomposition of the tensor into tensorial covariants*. This decomposition is generally not unique. Covariants $\mathbf{A}_a^{(\alpha)}$, $a = 1, 2, \ldots, n_\alpha$, must be linearly independent and can be replaced by a set of other linearly independent covariants $\mathbf{A}_b^{(\alpha)} = \sum_{b=1}^{n_\alpha} C_{ba} \mathbf{A}_a^{(\alpha)}$ [*cf.* relation (ii), §5]. The advantage of tensorial decomposition into covariants for consideration of transformation properties of a tensor under the action of the group G is quite clear. Instead of matrices $D^{(A)}(g)$ (*cf.* the end

Table 5
The four types of tensor according to their parity.

Type of tensor	Element of E_o e	i	e'	i'	Even rank	Odd rank
1_e^+ tensor	1	1	1	1	*i* tensor	*i* pseudotensor
1_e^- tensor	1	−1	1	−1	*i* pseudotensor	*i* tensor
1_m^+ tensor	1	1	−1	−1	*c* tensor	*c* pseudotensor
1_m^- tensor	1	−1	−1	1	*c* pseudotensor	*c* tensor

Table 6
The four types of scalars according to their parities.

Our symbol	Our name	Action of inversions e	i	e'	i'	Former name
1	1_e^+ scalar	1	1	1	1	*i* scalar
ε	1_e^- scalar	1	−1	1	−1	*i* pseudoscalar
τ	1_m^+ scalar	1	1	−1	−1	*c* scalar
$\varepsilon\tau$	1_m^- scalar	1	−1	−1	1	*c* pseudoscalar

of §4) of high dimensions we can use matrices $D^{(\alpha)}(g)$ of standard ireps whose dimensions do not exceed three. This is particularly suitable for comparison of tensor properties of domain states. In addition, covariant components constitute the bases of ireps necessary in the consideration of ferroic phase transitions.

Calculation of tensorial covariants up to fourth rank has been performed by consecutive use of Clebsch–Gordan products for the 32 point groups (Kopský, 1979*a*,*b*). In the resulting tables, we found regularities whose recent analysis uncovered Opechowski's magic relations (Kopský, 2006*a*). These relations hold in their simple form only for our standard choices of ireps for groups of oriented Laue classes. As a result of these relations, it is sufficient to find tensorial decompositions only for groups G of proper rotations and for tensors of positive parities with respect to space and magnetic inversions i and e' (and hence also with respect to combined inversion i'). Tensorial decompositions of tensors of other parities under action of any of the groups of the oriented Laue class G are related to the mentioned decompositions by simple rules.

We shall first explain the principle of these relations and then close this section and the paper by an example in which the use of both Clebsch–Gordan products and magic relations will be illustrated.

1. *The splitting of transformation properties of tensors:* Transformation properties of each tensor under the action of the full magnetic group $\mathcal{SO}(3) \otimes E_o$ split into two independent parts:

(i) its transformation properties with respect to the group of proper rotations $\mathcal{SO}(3)$;

(ii) its transformation properties with respect to the full group of inversions E_o. This follows from the fact that the full magnetic group is a direct product of the group of proper rotations with the full inversion group.

2. *Intrinsic symmetries:* Transformation properties of a tensor with respect to the group $\mathcal{SO}(3)$ are completely defined by its intrinsic symmetry which is completely specified by the well known Jahn symbols (Jahn, 1949). Thus V is the Jahn symbol for a vector, $[V]^2$ for a symmetric second-rank tensor, $\{V\}^2$ for an antisymmetric second-rank tensor, $V[V]^2$ for a third-rank tensor symmetrized in two indices, $[[V]^2]^2$ for a fourth-rank tensor, symmetric with respect to an exchange of the first and second indices, of the third and fourth indices and with the exchange of the first and second pair of indices, and so on.

3. *The four types of tensors:* The elements of the full inversion group $E_o = \{e, i, e', i'\}$ classify tensors into four types. Whatever the tensor **A** and whichever of the inversions acts on it, the tensor either does not change at all or it changes its sign. See Table 5.

According to the usual and historical terminology, ordinary (polar) tensors are those whose components transform like products of the components of an ordinary vector. Since the ordinary vector itself changes its sign under the space inversion i, a tensor is polar if it is of odd rank and changes its sign under the space inversion i or if its rank is even and the tensor does not change the sign under the inversion i. A tensor is called axial (or a pseudotensor) if its rank is odd and the tensor does not change its sign under the space inversion i or if it is even and changes sign under the space inversion i. In our symbols, the superscript $+$ or $-$ simply denotes the parity of a tensor under the action of the space inversion i: $+$ means even parity, *i.e.* the tensor does not change its sign; $-$ means odd parity, *i.e.* the tensor changes its sign. Indices e and m denote even and odd parities of a tensor under the action of magnetic inversion e'. This was originally indicated by letters i and c before the tensor.

4. *The four scalars:* Scalar quantities are one-component quantities which do not change under the action of the group of proper rotations $\mathcal{SO}(3)$. There are four types of scalars that differ by their transformation properties under the action of the full inversion group $E_o = \{e, i, e', i'\}$, *i.e.* by their parities. It is shown in Table 6 how these scalars change under the action of inversions. The symbols and names we shall use are given in the first two columns and compared with names used in the literature in the last column.

Lemma 1. Apart from their physical meaning, there exist exactly four types of tensors to each intrinsic symmetry which have the same transformation properties under the action of the group $\mathcal{SO}(3)$ of proper rotations and one of the four different parities.

Proof. Let **A** be a tensor of a certain intrinsic symmetry which defines its transformation properties under the action of the group of proper rotations $\mathcal{SO}(3)$. Applying inversions, we check its parity. Multiplying this tensor by the four scalars, we obtain four tensors of the same intrinsic symmetry and of the same transformation properties under the group $\mathcal{SO}(3)$.

We may therefore assume that the tensor **A** is a 1_e^+ tensor. Then the tensors $\varepsilon\mathbf{A}$, $\tau\mathbf{A}$ and $\varepsilon\tau\mathbf{A}$ are the 1_e^- tensor, the 1_m^+ tensor and the 1_m^- tensor, respectively.

Table 7
Example of calculation with Clebsch–Gordan products and of the use of Opechowski's magic relations.

Group	x_1 $\mathsf{x}_2^2\ \mathsf{x}_3^2\ \mathsf{x}_4^2$ $x_1^2+y_1^2$	x_2 $\mathsf{x}_3\mathsf{x}_4$ $x_1y_1-y_1x_1$	x_3 $\mathsf{x}_2\mathsf{x}_4$ $x_1^2-y_1^2$	x_4 $\mathsf{x}_2\mathsf{x}_3$ $x_1y_1+y_1x_1$	(x_1, y_1) $\mathsf{x}_2(y_1, -x_1)$ $\mathsf{x}_3(x_1, -y_1)$ $\mathsf{x}_4(y_1, x_1)$
D_{4z}		P_2			(P_1, P_2)
$4_z2_x2_{xy}$	u_1+u_2		u_1-u_2	u_6	(u_4, u_5)
	$u_1=u_2$				
	u_3	$d_{31}+d_{32}$	d_{36}	$d_{31}-d_{32}$	$(d_{11}, d_{22})\ (d_{12}, d_{21})$
		d_{33}			$(d_{13}, d_{23})\ (d_{26}, d_{16})$
	$d_{14}-d_{25}$	$d_{15}+d_{24}$	$d_{14}+d_{25}$	$d_{15}-d_{24}$	(d_{35}, d_{34})
	$d_{14}=-d_{25}$				
		$A_{31}+A_{32}$	A_{36}	$A_{31}-A_{32}$	$(A_{11}, A_{22})\ (A_{12}, A_{21})$
		A_{33}			$(A_{13}, A_{23})\ (A_{26}, A_{16})$
	$A_{14}-A_{25}$	$A_{15}+A_{24}$	$A_{14}+A_{25}$	$A_{15}-A_{24}$	(A_{35}, A_{34})
	$A_{14}=-A_{25}$				
C_{4vz}	$d_{31}+d_{32}$		$d_{31}-d_{32}$	d_{36}	$(d_{22}, -d_{11})\ (d_{21}, -d_{12})$
$4_zm_xm_{xy}$	$d_{15}+d_{24}$	$d_{14}-d_{25}$	$d_{15}-d_{24}$	$d_{14}+d_{25}$	$(d_{34}, -d_{35})$
	d_{33}				$(d_{23}, -d_{13})\ (d_{16}, -d_{26})$
	$d_{31}=d_{32}$				
	$d_{15}=d_{24}$				
	$\pi_{31}+\pi_{32}$		$\pi_{31}-\pi_{32}$	π_{36}	$(\pi_{22}, -\pi_{11})\ (\pi_{21}, -\pi_{12})$
	$\pi_{15}+\pi_{24}$	$\pi_{14}-\pi_{25}$	$\pi_{15}-\pi_{24}$	$\pi_{14}+\pi_{25}$	$(\pi_{34}, -\pi_{35})$
	π_{33}				$(\pi_{23}, -\pi_{13})\ (\pi_{16}, -\pi_{26})$
	$\pi_{31}=\pi_{32}$				
	$\pi_{15}=\pi_{24}$				
$C_{4vz}(C_{2v})$	$d_{31}+d_{32}$		$d_{31}-d_{32}$	d_{36}	$(d_{22}, -d_{11})\ (d_{21}, -d_{12})$
$4'_zm_xm'_{xy}$	$d_{15}+d_{24}$	$d_{14}-d_{25}$	$d_{15}-d_{24}$	$d_{14}+d_{25}$	$(d_{34}, -d_{35})$
	d_{33}				$(d_{23}, -d_{13})\ (d_{16}, -d_{26})$
	$d_{31}=d_{32}$				
	$d_{15}=d_{24}$				
	$\pi_{31}-\pi_{32}$	π_{36}	$\pi_{31}+\pi_{32}$		$(\pi_{22}, \pi_{11})\ (\pi_{21}, \pi_{12})$
			π_{33}		$(\pi_{23}, \pi_{13})\ (\pi_{16}, \pi_{26})$
	$\pi_{15}-\pi_{24}$	$\pi_{14}+\pi_{25}$	$\pi_{15}+\pi_{24}$	$\pi_{14}-\pi_{25}$	(π_{34}, π_{35})
	$\pi_{31}=-\pi_{32}$				
	$\pi_{15}=-\pi_{24}$				

Lemma 2. Let G_o be the group of proper rotations and $\mathbf{A}$ a 1_e^+ tensor. The four tensors $\mathbf{A}$, $\varepsilon\mathbf{A}$, $\tau\mathbf{A}$ and $\varepsilon\tau\mathbf{A}$ transform in exactly the same manner under the action of G_o.

Lemma 3. Any 1_e^+ tensor $\mathbf{A}$ transforms in the same manner under the action of elements g, ig, $e'g$ and $i'g$.

Proof. Each element of the group $\mathcal{SO}(3) \otimes E_o$ can be written as $jg = gj$, where $g \in \mathcal{SO}(3)$ and $j \in E_o$. The four tensors of the same intrinsic symmetry can be written as $s\mathbf{A}$, where $\mathbf{A}$ is a 1_e^+ tensor and $s \in (1, \varepsilon, \tau, \varepsilon\tau)$. It is also $jg(s\mathbf{A}) = (js)(g\mathbf{A})$. In the case of Lemma 2, it is $j = e$ and hence $g(s\mathbf{A}) = s(g\mathbf{A})$. In the case of Lemma 3, it is $s = 1$ and hence $jg\mathbf{A} = g\mathbf{A}$.

We recommend the reader now to consult the tables of tensorial decompositions (Kopský, 2001, pp. 50–65, Table *D*) where tensorial covariants of the following tensors are listed for the 32 point groups: enantiomorphism ε (1_e^- scalar), polarization $\mathbf{P} - V$, strain tensor $\mathbf{u} - [V]^2$, gyrotropic tensor $\mathbf{g} - \varepsilon[V]^2$, piezoelectricity $\mathbf{d} - V[V]^2$, electrogyration $\mathbf{A} - \varepsilon V[V]^2$, elastic stiffness $\mathbf{s} - [[V]^2]^2 \sim \mathbf{Q}^s$ the elastooptical tensor and its antisymmetric part $\mathbf{q} - \{[V]^2\}^2$. Notice that tensors $\mathbf{P}$, $\mathbf{g}$ and $\mathbf{d}$ are 1_e^- tensors which change sign under space inversion, while $\mathbf{u}$, $\mathbf{A}$ and $\mathbf{s}$ are 1_e^+ tensors. The decomposition of the latter into tensorial covariants is therefore common for all groups, isomorphic with the proper rotation group and their decomposition under the action of the centrosymmetric groups is the same in terms of typical variables with positive parity. A pseudovector $\mathbf{p} \sim \varepsilon\mathbf{P}$, not given in these tables, is also a 1_e^+ tensor and will transform in the same way for all groups as for the group of proper rotations.

The 1_e^- tensors $\mathbf{P} \sim \varepsilon\mathbf{p}$, $\mathbf{g} \sim \varepsilon\mathbf{u}$ and $\mathbf{d} \sim \varepsilon\mathbf{A}$, so that they transform in the same way as corresponding 1_e^- tensors under the action of the proper rotation group.

The pseudoscalar ε and the two other scalars τ and $\varepsilon\tau$ transform like one of the variables x_1, x_2, x_3, x_4 for other groups isomorphic with the proper rotation group, like variables x_1^+, x_2^+, x_3^+, x_4^+ or x_1^-, x_2^-, x_3^-, x_4^- for nonparamagnetic groups isomorphic with centrosymmetric groups, and like variables x_{1e}, x_{2e}, x_{3e}, x_{4e} or x_{1m}, x_{2m}, x_{3m}, x_{4m} for paramagnetic noncentrosymmetric groups. These *transformation properties of scalars* are determined by the distribution of inversions over the proper rotations and they are recorded in the last column of Table 2 for all groups of the oriented Laue class $D_{4z} - 4_z2_x2_{xy}$. Under the action of the paramagnetic centrosymmetric group, the scalars always transform like variables x_{1e}^-, x_{1m}^+ and x_{1m}^-, respectively.

Using Lemma 1, we may express any tensor in one of the forms: $\mathbf{A}$, $\varepsilon\mathbf{A}$, $\tau\mathbf{A}$, $\varepsilon\tau\mathbf{A}$, where $\mathbf{A}$ is a 1_e^+ tensor. Each of the scalars transforms under the action of any of the groups like one of the one-dimensional typical variables. Hence it is sufficient to calculate the decomposition of tensor $\mathbf{A}$ for the proper rotation group, find the typical variable which represents the scalar under the action of the considered group and use Clebsch–Gordan products with this variable to find the decomposition of the considered tensor. This is the essence of *Opechowski's magic relations*.[2]

Tensorial decompositions also imply the allowed form of the tensor under the action of the considered group. Indeed, the first column of tables of covariants lists tensorial invariants. These are generally linear combinations of Cartesian components. To obtain the Cartesian form of the tensor, we have to set all covariants to zero. This results in a set of conditions which Cartesian components of an invariant tensor must satisfy. Invariant tensors are also related for groups of the same Laue class. Opechowski (1975) observed that certain related properties are allowed in the same number of symmetries and called them the *magic numbers*. Their existence also follows from the magic relations between tensor decompositions.

Example: Calculate the decomposition of piezoelectric tensor $\mathbf{d}$, electrogyration tensor $\mathbf{A}$ and piezomagnetic tensor π for the group $D_{4z} - 4_z 2_x 2_{xy}$. Using Opechowski's magic relations, find the decomposition of these tensors for groups $C_{4z} - 4_z m_x m_{xy}$ and $C_{4z}(C_{2v}) - 4'_z m_x m'_{xy}$.

Solution: At the top of Table 7, we write the Clebsch–Gordan table which is valid for all groups isomorphic with $D_{4z} - 4_z 2_x 2_{xy}$. In the first row, we write the tensorial covariants of polarization $\mathbf{P}$. Comparing products $P_i P_j$, we obtain ($\sim$ means transforms like): $u_1 + u_2 \sim P_1^2 + P_2^2 \sim x_1^2 + y_1^2 \sim \mathsf{x}_1$ and $u_3 \sim P_3^2 \sim \mathsf{x}^2 \sim \mathsf{x}_1$, $u_1 - u_3 \sim P_1^2 - P_2^2 \sim x_1^2 - y_1^2 \sim \mathsf{x}_3$, $u_6 \sim P_1P_2 + P_2P_1 \sim x_1y_1 + y_1x_1 \sim \mathsf{x}_4$ and $(u_4, -u_5) \sim P_3(P_2, -P1) \sim \mathsf{x}_2(y_1, -x_1)$. We write this into the table and continue as follows:

$$P_3(u_1+u_2) \sim d_{31} + d_{32} \sim \mathsf{x}_2,\ P_3u_3 \sim d_{33} \sim \mathsf{x}_2,$$
$$P_3u_6 \sim d_{36} \sim \mathsf{x}_3,\ P_3(u_1-u_2) \sim d_{31} - d_{32} \sim \mathsf{x}_4,$$
$$P_1u_4 - P_2u_5 \sim d_{14} - d_{25} \sim \mathsf{x}_1,\ P_1u_5 + P_2u_4 \sim d_{15} + d_{24} \sim \mathsf{x}_2,$$
$$P_1u_4 + P_2u_5 \sim d_{14} + d_{25} \sim \mathsf{x}_3,\ P_1u_5 - P_2u_4 \sim d_{15} - d_{24} \sim \mathsf{x}_4,$$

and all Clebsch–Gordan products

$$(P_1, P_2)(u_1+u_2) \sim (d_{11}+d_{12}, d_{21}+d_{22}),$$
$$(P_1, P_2)(u_1-u_2) \sim (d_{11}-d_{12}, -d_{21}+d_{22}),$$
$$(P_1, P_2)u_3 \sim (d_{13}, d_{23}),\ (P_1, P_2)u_6 \sim (d_{13}, d_{23}),$$
$$(P_1, P_2)u_3 \sim (d_{13}, d_{23}),\ P_3(u_4, -u_5) \sim (d_{35}, d_{34})$$

transform like (x_1, y_1).

We take the sum and difference of the first two covariants using the law that the linear combination of covariants of the same type is again the covariant of the same type and the common factor does not play a role to get the results written in the next block of the table assigned to the group $D_{4z} - 4_z 2_x 2_{xy}$.

Tensors $\mathbf{A}$ and π have the same intrinsic symmetry as the tensor $\mathbf{d}$. According to Lemma 1 or Lemma 2, all three tensors have the same decomposition under the action of the group $D_{4z} - 4_z 2_x 2_{xy}$. Tensor $\mathbf{A}$ is the 1_e^+ tensor.

The components π_{ij}, $i = 1, 2, 3$, $j = 1, 2, 3, 4, 5, 6$, of the piezomagnetic tensor π transform like products $M_i u_j$ of the components of magnetization $\mathbf{M}$ and strain tensor $\mathbf{u}$. Tensors $\mathbf{d}$ and π transform like $\varepsilon\mathbf{A}$ and $\varepsilon\tau\mathbf{A}$, respectively. The 1_e^- scalar ε transforms like x_2 under both groups $C_{4z} - 4_z m_x m_{xy}$ and $C_{4z}(C_{2v}) - 4'_z m_x m'_{xy}$, while 1_m^- scalar $\varepsilon\tau$ transforms like x_2 in the first, like x_4 in the second of these groups. We can read their tensorial decompositions from that of $\mathbf{A}$ almost immediately.

9. Conclusions

To attract the attention of potential readers, we used the proud phrase *modern tensor calculus* in the title leaving it to the reader to decide whether it is justified. In our opinion, the method is now at a stage suitable for textbooks and classroom exercises. In paper 2, we shall try to justify it by application to a rather exacting problem of tensor parameters of domain states and their distinction.

This work is part of project AVO 10100520 of the Czech Academy and has been supported by grant No. 202/04/0992 of the Czech Grant Agency. Thanks are due to Professor M. Nespolo, who gave the author the opportunity to present the results in lectures at the Summer School of the MaThCryst group in Nancy, and to the French Embassy in Prague (Service de coopération et d'action culturelle) for generous support of local expenses as well as to my friend Professor D. B. Litvin who took care of the accommodation.

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[2] Complete tables of oriented Laue classes with transformation properties of scalars, including the noncrystallographic classes, are available from the web pages of the MaThCryst group (http://www.lcm3b.uhp-nancy.fr/mathcryst/) and from the IUCr electronic archives (see footnote **1**).

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