been obtained for fields which only approximately satisfy Maxwell's equations, and have been obtained without requiring the polarizability to be small.

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General Connections for the Form of Property Tensors in the 122 Shubnikov Point Groups

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Abstract

The 122 Shubnikov point groups (SPGs) are obtained from the 32 ordinary crystallographic point groups (OPGs) by taking time inversion into account. Like the OPGs, the SPGs can be grouped into 11 Laue classes. Tensors can be invariant under space inversion (s tensors), time inversion (t tensors), space-time inversion (u tensors) or all three inversions (i tensors). The restrictions imposed on the form of a property tensor by the SPG of the material under consideration depend, for i tensors, only on the Laue class of the SPG. If these restrictions are known for an i tensor, the corresponding restrictions for s, t and u tensors of the same rank and internal symmetry can be written down immediately for all the 122 SPGs and for all orientations in which the SPG under consideration appears in the corresponding holohedry. These connections provide tests for the forms of tensors given in the literature. A number of corrections and of possible simplifications are pointed out. The results are illustrated by showing how the form of the i tensor describing linear electrogyration determines the form of the piezoelectric t tensor and the piezomagnetic s tensor for all 122 SPGs. Similarly, the form of the t tensor describing quadratic electrogyration is derived explicitly from the i tensor describing the piezooptic effect.

1. Introduction

The 32 ordinary point groups (OPGs) and the 122 Shubnikov point groups (SPGs) that are compatible with a periodic structure in all three space dimensions are often arranged in a two-dimensional table. Its six columns essentially correspond to the crystal systems. The monoclinic point groups (PGs) appear either in the first column together with the anorthic PGs or in the second together with the orthorhombic PGs or in both in different orientations. PGs having certain features in common are placed in the same row. One such arrangement is given in *International Tables for X-ray Crystallography* (1952); another, which differs in important details (*e.g.* $\bar{4}3m$ in the same row as $4mm$ not as $\bar{4}2m$), has been proposed by Grimmer (1980), who called it the periodic arrangement. It has three long columns with PGs in every row and three short columns for which PGs are lacking in the same rows. He showed that, in his arrangement, each long column has the same subgroup structure if subgroups appearing several times in different orientations are distinguished. The same holds for the subgroup structure in the short columns. Groups in a given row have certain structural features in common, *e.g.* having space inversion $\bar{1}$, time inversion $1'$ or space-time inversion $\bar{1}'$ among their elements or containing such inversions only in combination with rotations. In this paper it is shown that the restrictions demanded by the PG of a material for the form of the tensors describing its properties also have features in common for all PGs in a given row. These restrictions are expressed as usual for the components of the tensor in a right-handed orthogonal coordinate system with the same length unit on the three axes. Care is taken to define completely the orientation of these axes with respect to the orientations of the symmetry elements, which are expressed by the order of the entries in the Hermann-Mauguin symbol.

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Table 1. *The periodic arrangement of the ordinary point groups (OPGs)*

1	2	3		4	5	6	7	8	9
		p	m	Anorthic monoclinic$\|x_2$	Monoclinic$\|x_3$ orthorhombic	Tetragonal	Trigonal	Hexagonal	Cubic
1		A	A	1	2	4	3	6	23
2	s	A	D		m	$\bar{4}$		$\bar{6}$	
5	S	A	0	$\bar{1}$	$2/m$	$4/m$	$\bar{3}$	$6/m$	$m\bar{3}$
12		B	B	2	222	422	32	622	432
13	s	B	C	m	$mm2$	$4mm$	$3m$	$6mm$	$\bar{4}3m$
16	s	B	E		$m2m$	$\bar{4}2m$		$\bar{6}2m$	
16′	s	B	F		$2mm$	$\bar{4}m2$		$\bar{6}m2$	
22	S	B	0	$2/m$	mmm	$4/mmm$	$\bar{3}m$	$6/mmm$	$m\bar{3}m$

2. The periodic arrangement of point groups and its connection with the form of tensors

Table 1 lists the 32 OPGs, some of which are in several orientations. Column 1 gives the same number to the rows that will be used in a similar table of all SPGs. The OPGs are denoted in columns 4 to 9 by their Hermann–Mauguin symbols,* which also contain information about the orientation of symmetry axes and planes as given in Table 2.4.1 of *International Tables for Crystallography* (1983). Table 1 contains the OPGs in all orientations in which they appear in the corresponding holohedry given in row 5 for anorthic and monoclinic OPGs and in row 22 for OPGs in the other crystal systems. An S in column 2 indicates that the OPGs in the corresponding row contain space inversion $\bar{1}$, an s that $\bar{1}$ appears only in combination with a rotation. The letters A–F in column 3 give information about the form of tensors, as will be explained in detail later; 0 indicates a vanishing tensor.

In order to describe tensors, the following right-handed orthonormal coordinate systems will be used: for cubic crystals, x_1, x_2 and x_3 are in directions corresponding to the first entry in the Hermann–Mauguin symbol; for tetragonal, trigonal and hexagonal crystals, x_3 is in a direction corresponding to the first entry and x_1 in a direction corresponding to the second entry. (If there is no second entry then x_1 may be any direction perpendicular to x_3.) For orthorhombic crystals x_1 is in the direction of the first entry, x_2 of the second and x_3 of the third. The monoclinic axis is chosen in the direction of x_2 in column 4 and in the direction of x_3 in column 5. For anorthic crystals, any right-handed orthonormal system may be chosen. Using these conventions, the tensors take the form implied by the *IEEE Standard on Piezoelectricity* (1978) if the monoclinic axis is chosen parallel to x_2 and if the other point groups that appear more than once are chosen in the orientations $mm2$, $\bar{4}2m$ and $\bar{6}2m$.†

The number of indices of a tensor is called its rank r. The tensor may show interior symmetry if it remains invariant or changes sign under certain permutations of its indices. Tensors transform as products of r coordinates under rotations; under roto-inversions, *i.e.* rotations combined with $\bar{1}$, the tensor may change sign in addition. Tensors of even rank that remain invariant under $\bar{1}$ and tensors of odd rank that change sign under $\bar{1}$ are usually called polar tensors; tensors of even rank that change sign and tensors of odd rank that remain invariant under $\bar{1}$ are then called axial tensors. It is more convenient for a discussion of formal properties to call any tensor that remains invariant under $\bar{1}$ a (plus or) p tensor and one that changes sign a (minus or) m tensor.

Tensors describing properties of materials (called 'property' or 'material' tensors) are invariant under the elements of the PG of the material. Attention will be restricted in the following to such tensors. The PGs in rows 5 and 22 contain $\bar{1}$. They will be called Laue groups. Because m tensors change sign under $\bar{1}$ they must vanish for the 11 Laue groups. The number 0 appears therefore on the right side of column 3 for the Laue groups. It follows that m tensors of any rank can be different from zero for at most 21 of the 32 OPGs. If the PG contains only rotations (rows 1 and 12), there are obviously the same restrictions for p and m tensors. The same letter (A in row 1, B in row 12) appears therefore in both subcolumns 3. Two OPGs that together with $\bar{1}$ generate the same Laue group, are said to belong to the same Laue class. The OPGs in any of the columns 4–9 fall into two Laue classes; the OPGs above the horizontal line belong to one Laue class, those below to the other. Because a p tensor is invariant under $\bar{1}$, the restrictions imposed on it by an OPG depend only on its Laue class. This is the reason why, on the left side of column 3, A appears in all rows above the

* Grimmer (1980) deviated from the usual Hermann–Mauguin conventions by interchanging the first and third entries for orthorhombic PGs in order to make the analogy between columns 5, 6 and 8 evident. We return in the present paper to the usual Hermann–Mauguin conventions.

† $\bar{6}2m$ is called $\bar{6}m2$ in the *IEEE Standard on Piezoelectricity* (1978), deviating in this case from the international conventions on the orientation of the symmetry elements in the Hermann–Mauguin symbol.

line and B in all rows below. This completes the proof that the restrictions on the form of material tensors have the structure indicated in column 3.

It will be shown that the forms C, D, E and F can be deduced immediately from A and B. Let $A+B$ denote a tensor that can be written as the sum of two tensors satisfying the restrictions A and B, respectively, and $A\cap B$ a tensor that simultaneously satisfies the restrictions A and B. The group in rows 12 and 13 in the same column have the group in row 1 in common and generate together the group in row 22. Similarly, the groups in rows 16 and 16′ of the same column have the group in row 2 in common and generate together the group in row 22. A tensor that satisfies the restrictions B and C or E and F must vanish therefore, $B\cap C=0$ and $E\cap F=0$. The sum $B+C$ will satisfy the restrictions A, *i.e.* $A\supseteq B+C$, similarly, $D\supseteq E+F$. Let n_A denote the number of independent components of a tensor of form A in the column under consideration. We shall show $n_A=n_B+n_C$ and $n_D=n_E+n_F$, from which it follows that $A=B+C$ and $D=E+F$ because $B\cap C=0$ and $E\cap F=0$.

The groups in rows 1 and 2 in the same column generate together the group in row 5; they have a group in row 1 in common that belongs to another column with half as many elements in its groups (column 4 instead of 5, 5 instead of 6 and 7 instead of 8). The groups in rows 12 and 16 generate together the group in row 22; they have the group in row 12 of the neighbouring column to the left in common, as above. Similarly, the groups in rows 13 and 16′ generate together the group in row 22; they have the group in row 13 of the neighbouring column to the left in common. Because m tensors vanish for the groups in the rows 5 and 22, we conclude that $A\cap D=0$, $B\cap E=0$ and $C\cap F=0$. As above, one finds that $A'\supseteq A+D$, $B'\supseteq B+E$ and $C'\supseteq C+F$, where A' refers to columns 4, 5 or 7 if A refers to columns 5, 6 or 8, respectively. We shall show $n_{A'}=n_A+n_D$, $n_{B'}=n_B+n_E$ and $n_{C'}=n_C+n_F$, from which it follows that $A'=A+D$ because $A\cap D=0$ and, similarly, that $B'=B+E$ and $C'=C+F$. Because $A'=A+D$ and $A\cap D=0$, the form D is determined uniquely if the forms A and A' are known, so that we can write $D=A'-A$ and similarly $E=B'-B$, $F=C'-C$. From $A=B+C$ and $B\cap C=0$ it follows that $C=A-B$, so that all the forms C, D, E and F can be expressed in terms of forms of types A and B.

The number of independent components of a tensor in a material with point group G having elements g_i, $i=1,\ldots,N$, is given by

$$n=(1/N)\sum_{i=1}^{N}\chi(g_i), \qquad (1)$$

where $\chi(g_i)$ is the character of the element g_i in the representation corresponding to the tensor under consideration.* Consider as an example (1) for a given m tensor and the three point groups 6, 622 and $6mm$. Six of the twelve elements of $6mm$ are rotations that appear also in 622. They form the group 6. The six other elements of $6mm$ are the six other rotations of 622 followed by $\bar{1}$. Denote by r_i, $i=1,\ldots,6$, the rotations in the group 6, by r_i, $i=7,\ldots,12$, the rotations in 622 but not in 6. Then,

$$n_{622}=\tfrac{1}{12}\left[\sum_{i=1}^{6}\chi(r_i)+\sum_{i=7}^{12}\chi(r_i)\right],$$

$$n_{6mm}=\tfrac{1}{12}\left[\sum_{i=1}^{6}\chi(r_i)-\sum_{i=7}^{12}\chi(r_i)\right],$$

$$n_6=\tfrac{1}{6}\sum_{i=1}^{6}\chi(r_i).$$

It follows that $n_6=n_{622}+n_{6mm}$. A similar argument holds for the groups in the same rows but a different column (4–9) of Table 1, giving $n_A=n_B+n_C$. The proofs that $n_D=n_E+n_F$, $n_{A'}=n_A+n_D$, $n_{B'}=n_B+n_E$, $n_{C'}=n_C+n_F$ follow along the same lines. Notice that $n_E=n_F$, *i.e.* n_D is always even.†

3. An example: tensors of third rank symmetric in two of their three indices

The optical activity of a crystal can appear or change in an electric field $\mathbf{E}$:

$$g_{jk}(\mathbf{E})=g^0_{jk}+A_{ijk}E_i+B_{jklm}E_lE_m+\ldots, \qquad (2)$$

where $\mathbf{g}^0$ is the gyration tensor in the absence of a field (see *e.g.* Shuvalov, 1988). The tensor $\mathbf{g}$ may be considered symmetric (see *e.g.* Nye, 1957), whence the tensor $\mathbf{A}=A_{ijk}$ of linear electrogyration is symmetric in its last two indices and the tensor $\mathbf{B}=B_{jklm}$ of quadratic electrogyration is symmetric in its first two and its last two indices. Because $\mathbf{g}$ and $\mathbf{E}$ are of type m, $\mathbf{A}$ will be of type p and $\mathbf{B}$ of type m. The

* The traditional presentation, most clearly given by Niggli (1955), starts by considering polar tensors only. The number of independent components is then given by

$$n=(1/N)\sum_{i=1}^{N}\chi(g_i)\chi_j(g_i),$$

where χ is the character of a polar representation and χ_j the character of the totally symmetric representation ($\chi_j\equiv 1$) for polar tensors and of the antisymmetric representation ($\chi_j=1$ for rotations and $\chi_j=-1$ for roto-inversions) for axial tensors. It seems that the current presentation is not only simpler but also logically more satisfactory. It should be stressed, however, that the remainder of this paper does not depend on whether the reader adopts the author's point of view or prefers the traditional one.

† These results give general proofs of regularities that one may observe in the tables of Niggli (1955) and indicate how the tables could be written more compactly. The results show also that a correction is needed in his Table 5, where 1 instead of 0 should appear on the left side (A') of column $\bar{4}3m$ in the rows $3(3m-A')$, $3(3\text{-}A)$, $3(m\text{-}A')$ and $3(1-A)$.

form of the fourth-rank tensor **B** for the various point groups will be given in § 5 (Fig. 2).

A crystal may develop an electric polarization **P** if it is subject to a stress $\boldsymbol{\sigma}$,

$$P_i = d_{ijk}\sigma_{jk}.$$

The tensor $\boldsymbol{\sigma}$ being symmetric, the piezoelectric tensor d_{ijk} can also be chosen symmetric in its last two indices (see e.g. Nye, 1957). Because **P** is of type *m* and $\boldsymbol{\sigma}$ of type *p*, **d** will be of type *m*.

A third-rank tensor T_{ijk} that is symmetric in its last two indices can be expressed by a matrix if the last two indices are replaced as follows by a single one running from 1 to 6:

$$\begin{array}{ccccccc} \mu & 1 & 2 & 3 & 4 & 5 & 6 \\ j,k & 1,1 & 2,2 & 3,3 & 2,3 & 3,1 & 1,2 \end{array} \qquad (3)$$

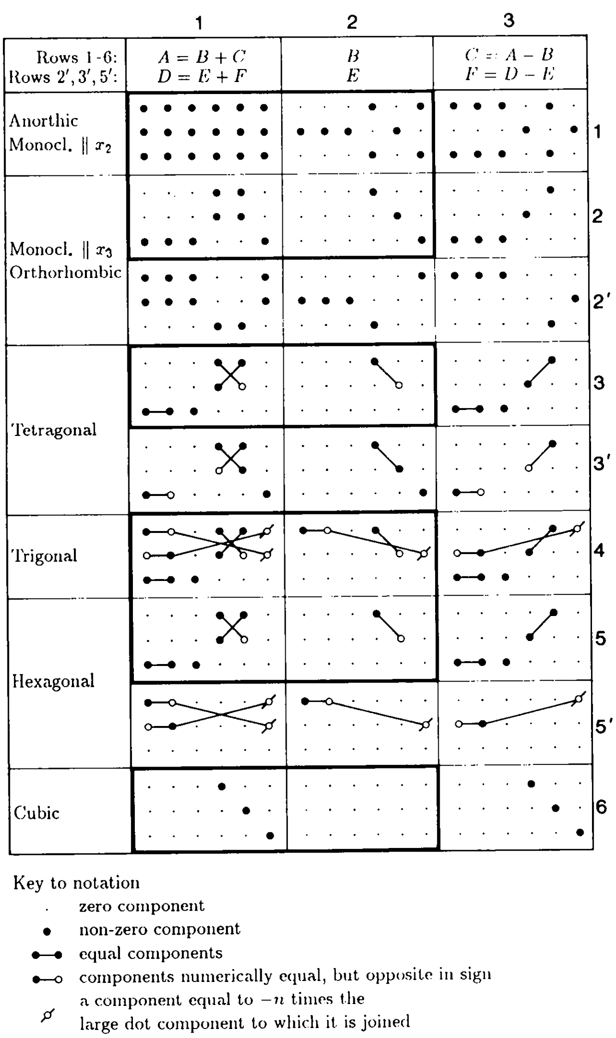

Fig. 1. Form of the matrices for third-rank tensors, symmetric in two of their three indices. The thicker boxes contain the matrices *A* and *B*, which appear for *i* tensors and determine the other matrices.

This reduces the number of components from $3^3 = 27$ to $3\times 6 = 18$. In order to maintain the convention of summation over repeated indices in passing from $A_i = T_{ijk}B_{jk}$ to $A_i = T_{i\mu}B_\mu$ the factor 2 has to be introduced in either **B** or in **T**:

$$\begin{aligned} T_{i\mu} &= T_{ijk} \text{ for } \mu = 1, 2 \text{ or } 3, \\ T_{i\mu} &= nT_{ijk} \text{ for } \mu = 4, 5 \text{ or } 6, \end{aligned} \qquad (4)$$

where $n = 1$ if the factor 2 has been incorporated in the definition of **B** and $n = 2$ otherwise. Usually, one puts $n = 2$ for **d** (see *e.g.* Nye, 1957) and **A** (see *e.g.* Zheludev, 1978; Landolt-Börnstein, 1984).* With this matrix notation, the letters *A*–*F* of Table 1 take the meanings given in Fig. 1. It shows that, for each row, the matrix in column 1 can be written as a sum of the matrices in columns 2 and 3 and that the matrices in columns 2 and 3 have only the zero matrix in common, illustrating our general results $A = B + C$, $D = E + F$ and $B\cap C = 0$, $E\cap F = 0$. Similarly, one finds that for each column the matrices in rows 2 and 2′ (3 and 3′, 5 and 5′) have only the matrix 0 in common and that their sum has the form of the matrix in row 1 (2, 4), illustrating again general results derived in the preceding section.

Fig. 1 gives the form of the matrices simultaneously for linear electrogyration, piezoelectricity and piezomagnetism. They are given separately for piezoelectricity in Landolt-Börnstein (1979)† and for linear electrogyration in Landolt-Börnstein (1984).‡

4. The restrictions put on material tensors by the 122 Shubnikov point groups

The extension of Table 1 from the 32 OPGs to all 122 SPGs is given in Table 2.

The capital letters *S*, *T* and *U* in column 2 indicate that the SPGs in the corresponding rows contain space inversion $\bar{1}$, time inversion 1′ and space-time inversion $\bar{1}'$, respectively. Small letters *s*, *t* and *u* indicate that the groups contain these inversions only combined with non-trivial rotations (*i.e.* different from the identity 1).

Tensors may be invariant or change sign under $\bar{1}$, 1′, $\bar{1}'$. If $\bar{1}$ is followed or preceded by 1′ then $\bar{1}'$ is obtained. Hence if the tensor changes sign under $\bar{1}$ and 1′ it must be invariant under $\bar{1}'$. Considerations of this type limit the number of possible combinations of invariance and sign changes from 16 to 4. These four combinations correspond to the four irreducible

* Notice that $n = 2$ amounts to defining $g_\mu = 2g_{jk}$ if $\mu = 4$, 5 or 6 when *jk* is replaced by μ in (2).

† Landolt-Börnstein (1979, 1984) follows the *IEEE Standard on Piezoelectricity* (1978) in writing $\bar{6}m2$ for an orientation of the group that is denoted by $\bar{6}2m$ according to the international conventions.

‡ In Table *S*2, η_{61} and η_{62} should be replaced by 0 in Laue class $2/m$; η_{41} and $2\eta_{11}$ by $-\eta_{41}$ and $-2\eta_{11}$ in Laue class $\bar{3}m$.

Table 2. *The periodic arrangement of the Shubnikov point groups (SPGs)*

1	2			3				4	5	6	7	8	9
				i	*s*	*t*	*u*	Anorthic Monoclinic	Monoclinic Orthorhombic	Tetragonal	Trigonal	Hexagonal	Cubic
1				*A*	*A*	*A*	*A*	1	2	4	3	6	23
2	*s*			*A*	*A*	*D*	*D*		m	$\bar{4}$		$\bar{6}$	
3		*t*		*A*	*D*	*A*	*D*		$2'$	$4'$		$6'$	
4			*u*	*A*	*D*	*D*	*A*		m'	$\bar{4}'$		$\bar{6}'$	
5	*S*			*A*	*A*			$\bar{1}$	$2/m$	$4/m$	$\bar{3}$	$6/m$	$m\bar{3}$
6		*T*		*A*		*A*		$11'$	$21'$	$41'$	$31'$	$61'$	$231'$
7			*U*	*A*			*A*	$\bar{1}'$	$2/m'$	$4/m'$	$\bar{3}'$	$6/m'$	$m'\bar{3}'$
8	*S*	*t*	*u*	*A*	*D*				$2'/m'$	$4'/m$		$6'/m'$	
9	*s*	*T*	*u*	*A*		*D*			$m1'$	$\bar{4}1'$		$\bar{6}1'$	
10	*s*	*t*	*U*	*A*			*D*		$2'/m$	$4'/m'$		$6'/m$	
11	*S*	*T*	*U*	*A*				$\bar{1}1'$	$2/m1'$	$4/m1'$	$\bar{3}1'$	$6/m1'$	$m\bar{3}1'$
12				*B*	*B*	*B*	*B*	2	222	422	32	622	432
13	*s*			*B*	*B*	*C*	*C*	m	$mm2$	$4mm$	$3m$	$6mm$	$\bar{4}3m$
14		*t*		*B*	*C*	*B*	*C*	$2'$	$2'2'2$	$42'2'$	$32'$	$62'2'$	$4'32'$
15			*u*	*B*	*C*	*C*	*B*	m'	$m'm'2$	$4m'm'$	$3m'$	$6m'm'$	$\bar{4}'3m'$
16	*s*			*B*	*B*	*E*	*E*		$m2m$	$\bar{4}2m$		$\bar{6}2m$	
17		*t*		*B*	*E*	*B*	*E*		$2'22'$	$4'22'$		$6'22'$	
18			*u*	*B*	*E*	*E*	*B*		$m'2m'$	$\bar{4}'2m'$		$\bar{6}'2m'$	
19	*s*	*t*	*u*	*B*	*C*	*E*	*F*		$m'2'm$	$\bar{4}2'm'$		$\bar{6}2'm'$	
20	*s*	*t*	*u*	*B*	*F*	*C*	*E*		$mm'2'$	$4'm'm$		$6'm'm$	
21	*s*	*t*	*u*	*B*	*E*	*F*	*C*		$2'mm'$	$\bar{4}'m2'$		$\bar{6}'m2'$	
22	*S*			*B*	*B*			$2/m$	mmm	$4/mmm$	$\bar{3}m$	$6/mmm$	$m\bar{3}m$
23		*T*		*B*		*B*		$21'$	$2221'$	$4221'$	$321'$	$6221'$	$4321'$
24			*U*	*B*			*B*	$2/m'$	$m'm'm'$	$4/m'm'm'$	$\bar{3}'m'$	$6/m'm'm'$	$m'\bar{3}'m'$
25	*S*	*t*	*u*	*B*	*C*			$2'/m'$	$m'm'm$	$4/mm'm'$	$\bar{3}m'$	$6/mm'm'$	$m\bar{3}m'$
26	*s*	*T*	*u*	*B*		*C*		$m1'$	$mm21'$	$4mm1'$	$3m1'$	$6mm1'$	$\bar{4}3m1'$
27	*s*	*t*	*U*	*B*			*C*	$2'/m$	mmm'	$4/m'mm$	$\bar{3}'m$	$6/m'mm$	$m'\bar{3}'m$
28	*S*	*t*	*u*	*B*	*E*				$m'mm'$	$4'/mmm'$		$6'/m'mm'$	
29	*s*	*T*	*u*	*B*		*E*			$m2m1'$	$\bar{4}2m1'$		$\bar{6}2m1'$	
30	*s*	*t*	*U*	*B*			*E*		$mm'm$	$4'/m'm'm$		$6'/mm'm$	
31	*S*	*T*	*U*	*B*				$2/m1'$	$mmm1'$	$4/mmm1'$	$\bar{3}m1'$	$6/mmm1'$	$m\bar{3}m1'$

Table 3. *The four tensor types defined by their behaviour under inversions*

1	$\bar{1}$	$1'$	$\bar{1}'$	Tensor type
1	1	1	1	*i* tensor, invariant under all inversions
1	1	−1	−1	*s* tensor, invariant under space inversion
1	−1	1	−1	*t* tensor, invariant under time inversion
1	−1	−1	1	*u* tensor, invariant under space-time inversion

representations of the group formed by $\bar{1}$, $1'$, $\bar{1}'$ and 1. The combinations are given in Table 3, where sign change is denoted by −1 and invariance by 1.

Material tensors are invariant under the transformations contained in the SPG of the material. It follows that *s* tensors vanish for SPGs containing $1'$ or $\bar{1}'$ (marked *T* or *U*, respectively, in column 2 of Table 2); *t* tensors vanish for groups marked *U* or *S* and *u* tensors for groups marked *S* or *T*. The vanishing of a tensor is marked by a blank space in column 3 of Table 2 instead of the 0 used in Table 1. Tensors of type *s*, *t* or *u* can be different from zero in (at the most) 69 of the 122 SPGs.

Similar methods to those used for determining the distribution of the forms $A-F$ in column 3 of Table 1 determine also their distribution in the corresponding column of Table 2 and show that no additional forms appear. The OPGs correspond to the rows without *T*, *U*, *t* or *u* in column 2. For these groups the same restrictions hold for *i* and *s* tensors because both are invariant under $\bar{1}$ and there are the same restrictions for *t* and *u* tensors, which change sign under $\bar{1}$. The same letters therefore appear in the first two and in the last two subcolumns 3 for the rows containing OPGs; a *p* tensor may be of either *i* or *s* type, depending on its behaviour under time inversion, and an *m* tensor may be of either *t* or *u* type.

The 7 holohedries and the 11 Laue groups are redefined to contain also $1'$, *i.e.* they are now given in rows 11 and 31 instead of 5 and 22. Two SPGs that together with $\bar{1}$ and $1'$ generate the same Laue group are put into the same Laue class. All SPGs in rows 1-11 of a given column belong to one and the same Laue class and the ones in rows 12-31 to another. The restrictions imposed on the form of an *i* tensor by the SPG depend only on its Laue class. They are marked *A* or *B*. It was shown in the last section how the restrictions *C*-*F* follow from them. Therefore, if the form of an *i* tensor is known for the 11 Laue classes (for both orientations of the monoclinic Laue class) we can immediately give the form of the corresponding *s*, *t* and *u* tensors for all 122 SPGs.

The first and second entries of the Hermann-Mauguin symbol differ in the rows 16-21 and 28-30 of column 5. In columns 6 and 8 the second and third

Table 4. *Comparison between the symbols A–U employed by Birss (1964) and the symbols A–F of the present paper*

	A	*B*	*C*	*D*	*E*	*F*
Anorthic/monoclinic$\|x_2$	*A*					
Monoclinic$\|x_3$/orthorhombic	*B*	*D*	*E*	*C*		
Tetragonal	*F*	*H*	*I*	*G*	*J*	
Trigonal	*K*	(*L*)	(*M*)			
Hexagonal	*N*	*P*	*Q*	*O*		*R*
Cubic	*S*	*T*	*U*			

Table 5. *Correspondence between the four types of tensors distinguished in this paper and the eight types of Birss* (1964)

This paper	Birss	
	Rank even	Rank odd
i tensor	Polar *i* tensor	Axial *i* tensor
s tensor	Polar *c* tensor	Axial *c* tensor
t tensor	Axial *i* tensor	Polar *i* tensor
u tensor	Axial *c* tensor	Polar *c* tensor

entries differ in the same rows. If these entries are exchanged then *E* has to be replaced by *F* and *F* by *E* in column 3. This procedure gives rows 16′–21′ and 28′–30′. If we add them to Table 2 (*cf.* row 16′ in Table 1), then the table will contain the SPGs in all orientations in which they appear in the corresponding holohedry.

Let us reconsider the example of § 3. The electrogyration tensor **A** is of type *i* and **B** of type *t*. Also, the piezoelectric tensor **d** is of type *t*. A crystal that is subject to a stress $\boldsymbol{\sigma}$ may develop also a magnetization **I** (see *e.g.* Birss, 1964),

$$I_i = Q_{ijk}\sigma_{jk}.$$

As for the piezoelectric tensor d_{ijk}, the piezomagnetic tensor Q_{ijk} can be chosen symmetric in its last two indices. The indices *j*, *k* are again replaced by a single index μ, running from 1 to 6. Because **I** is of type *s* and $\boldsymbol{\sigma}$ of type *i*, **Q** will be of type *s*, too.* The form of **Q** in the 122 SPGs is obtained from Table 2 and Fig. 1.

5. Discussion and illustration of the results

Birss (1964) also uses in his Tables 4*a* and 7 letters to indicate the form of property tensors in the 122 SPGs. The connection between his letters *A–U* and our letters *A–F* is given in Table 4.

The present paper follows Nye (1957) and Landolt-Börnstein (1979, 1984) in choosing the orientation of the orthogonal axes x_1, x_2, x_3 relative to the symmetry axes of the material in a way compatible with the IEEE standard. For comparison, the orthogonal axes used by Birss differ from ours for trigonal crystals by a 30° rotation about the principal symmetry axis. This is the reason why our trigonal *A* is split differently by his *L* and *M* than by our trigonal *B* and *C*.

There are a number of further differences between Birss's and the present approach:

1. Birss does not note the connections between different forms, which allowed us to express the forms *C*, *D*, *E* and *F* in terms of *A* and *B*.

* The behaviour of vectors under $\bar{1}$, 1′ and $\bar{1}'$ has been discussed by Ascher (1974).

2. Whereas in the present paper the orientation of the tensor indicated by the letter symbol always corresponds to the orientation indicated by the Hermann–Mauguin symbol, Birss (1964) has to use brackets in his Table 7 in order to mark the cases in which the two orientations do not agree. The reason for this can be seen from our Tables 2 and 4. Birss uses a minimal set of different forms, 21 instead of 27, as shown in Table 4. Take as an example our orthorhombic form *C* (form *E* of Birss). Table 2 shows that it describes the form of an *s* tensor for $m'2'm$ (and $2'm'm$), of a *t* tensor for $mm'2'$ (and $m'm2'$) and of a *u* tensor for $2'mm'$ (and $m2'm'$), which denote the same SPG in six different orientations. Birss considers this point group only in the orientation $2'm'm$ in his Table 7. This is the reason why he has to write (*E*) in the case of *t* and *u* tensors.*

3. Birss only considers the 90 'magnetic' point groups, omitting the 32 'grey' SPGs, which are contained in the rows marked *T* in column 2 of Table 2.

4. Birss calls a tensor of rank *m* 'polar' if it transforms under rotations and rotations combined with $\bar{1}$ (roto-inversions) as a product of *m* coordinate vectors and 'axial' if an additional sign change occurs for roto-inversions. According to whether a tensor remains invariant or changes sign under 1′ he calls it an *i* or a *c* tensor. He arrives in this way at eight types of tensors that pairwise correspond to our four types, as indicated in Table 5.

The present approach simplifies the presentation of the results and makes it evident that $\bar{1}$, 1′ and $\bar{1}'$ play an analogous role in the point groups. It makes evident also the analogous behaviour of the SPGs in the various columns of Table 2.

Some authors who, in a similar fashion to Birss, use a minimal set of different forms and the Hermann–Mauguin symbols with entries only in some definite order do not care about the agreement of the orientations. This is a source of much confusion in the published literature.

The decisive advantages of the present method are listed in points 1 and 2: they allow the use of the

* Brackets are lacking around *R* in his Table 7 in the two columns corresponding to *t* tensors for $\bar{6}'2m'$ and in the two columns corresponding to *u* tensors for $\bar{6}m'2'$.

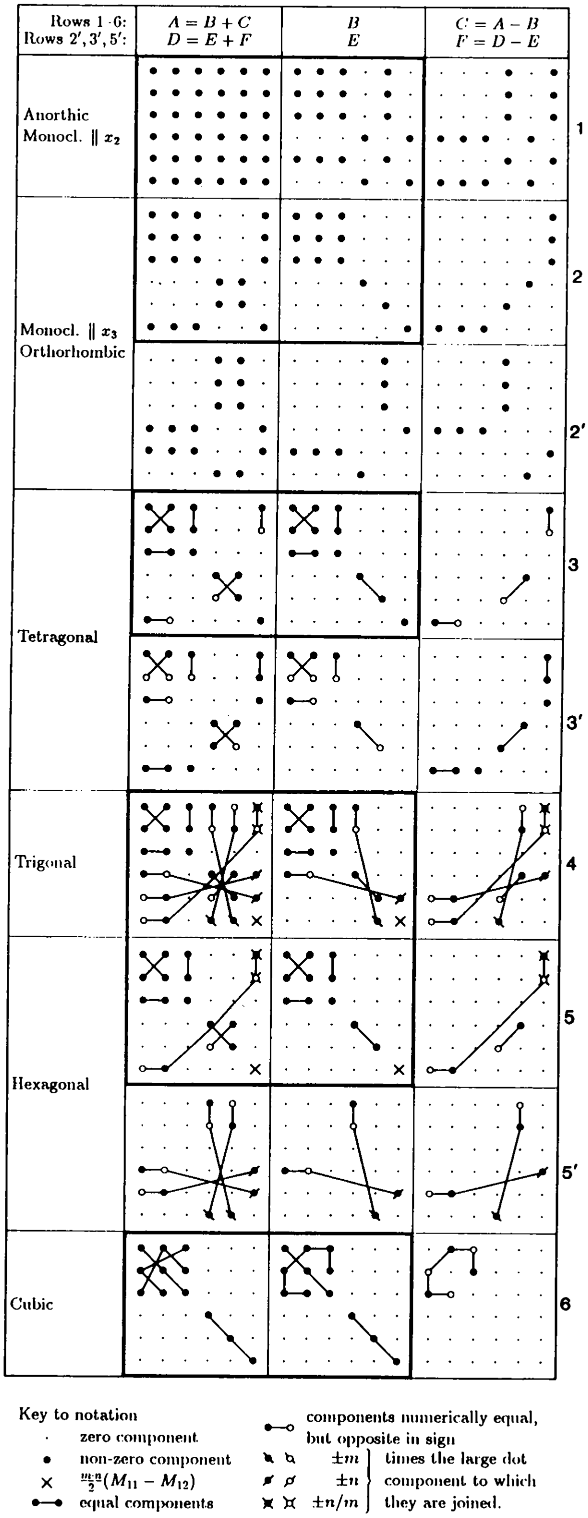

Fig. 2. Form of the matrices for fourth-rank tensors, symmetric in the first and second pairs of indices. The thicker boxes contain the matrices A and B, which appear for i tensors and determine the other matrices. (M_{11} denotes the element in the upper left corner of the matrix, M_{12} its neighbour to the right.)

numerous results available on the forms of i tensors in order to write down the forms of the corresponding s, t and u tensors. Take as an example the form of the elasto-optic tensor p_{ijkl}, which expresses $\Delta\beta$, the change in the dielectric impermeability at optical frequencies, in terms of the strains. This tensor is of type i and is symmetric with respect to the first and the second pairs of indices. Each pair is replaced by a single index running from 1 to 6 in order to express the tensor by a matrix, *i.e.* $ij \to \mu$ and $kl \to \nu$, as in (3). This reduces the number of components from $3^4 = 81$ to $6^2 = 36$. The price that one has to pay is the introduction of factors similar to (4):

$$T_{\mu\nu} = T_{ijkl} \quad \text{if } \mu = 1, 2 \text{ or } 3 \text{ and } \nu = 1, 2 \text{ or } 3,$$

$$T_{\mu\nu} = mT_{ijkl} \quad \text{if } \mu = 4, 5 \text{ or } 6 \text{ and } \nu = 1, 2 \text{ or } 3,$$

$$T_{\mu\nu} = nT_{ijkl} \quad \text{if } \mu = 1, 2 \text{ or } 3 \text{ and } \nu = 4, 5 \text{ or } 6,$$

$$T_{\mu\nu} = mnT_{ijkl} \quad \text{if } \mu = 4, 5 \text{ or } 6 \text{ and } \nu = 4, 5 \text{ or } 6,$$

where m and n are either 1 or 2. With the usual definitions, $m = n = 1$ for the elasto-optic coefficients $p_{\mu\nu}$ and $m = 1$, $n = 2$ for the piezo-optic coefficients $q_{\mu\nu}$, which express $\Delta\beta$ in terms of the strains and the stresses, respectively. The forms of these coefficients have been listed *e.g.* by Nye (1957) and Landolt-Börnstein (1979). With the form types A and B known, the types C, D, E and F can be deduced as shown in Fig. 2. Together they give the matrices describing quadratic electrogyration. To the author's knowledge, these matrices are published here for the first time. Notice that all form types in Fig. 2 are different and different from 0. It follows that quadratic electrogyration can appear in all 21 non-centrosymmetric OPGs; it has been found experimentally in quartz (see Zheludev, 1978).

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