FIESCHI, R. & FUMI, F. G. (1953). *Nuovo Cimento*, **10**, 865–882.
FUMI, F. G. (1951). *Phys. Rev.* **83**, 1274–1275.
FUMI, F. G. (1952*a*). *Acta Cryst.* **5**, 44–48.
FUMI, F. G. (1952*b*). *Acta Cryst.* **5**, 691–694.
FUMI, F. G. (1952*c*). *Nuovo Cimento*, **9**, 739–756.
FUMI, F. G. (1952*d*). *Phys. Rev.* **86**, 561.
FUMI, F. G. & RIPAMONTI, C. (1980). *Acta Cryst.* A**36**, 551–558.
GREEN, A. E. & ADKINS, J. E. (1960). *Large Elastic Deformations*. Oxford: Clarendon Press.
HEARMON, R. F. S. (1961). *An Introduction to Applied Anisotropic Elasticity*. Oxford University Press.
HEINE, V. (1960). *Group Theory in Quantum Mechanics*. London: Pergamon Press.
HERMANN, C. (1934). *Z. Kristallogr.* **89**, 32–48.
JAGODZINSKI, H. & WONDRATSCHEK, H. (1955). *Handbuch der Physik*. Vol. VII. 1, pp. 40–59. Berlin: Springer.
JAHN, H. A. (1937). *Z. Kristallogr.* **98**, 191–200.
JURETSCHKE, H. J. (1975). *Crystal Physics*. Reading, Mass.: Addison Wesley.
LANDAU, L. & LIFSHITZ, E. (1959). *Theory of Elasticity*, 1st ed. London & Paris: Pergamon Press.
LANDAU, L. & LIFSHITZ, E. (1960). *Electrodynamics of Continuous Media*, 1st ed. London & Paris: Pergamon Press.
LAX, M. (1974). *Symmetry Principles in Solid State and Molecular Physics*. New York: John Wiley.
MASON, W. P. (1966). *Crystal Physics of Interaction Processes*. New York: Academic Press.
MURNAGHAN, F. D. (1951). *Finite Deformation of an Elastic Solid*. New York: John Wiley.
NEUMANN, F. (1885). *Vorlesungen über die Theorie der Elastizität*. Leipzig: Teubner.
NOWICK, A. S. & HELLER, W. R. (1965). *Adv. Phys.* **14**, 101–166.
NYE, J. F. (1957). *Physical Properties of Crystals*. Oxford: Clarendon Press.
SCHOUTEN, J. A. (1951, 1954). *Tensor Analysis for Physicists*, 1st & 2nd eds. Oxford: Clarendon Press.
SIROTIN, YU. I. (1960). *Sov. Phys. Crystallogr.* **5**, 157–165.
SIROTIN, YU. I. (1961). *Sov. Phys. Dokl.* **5**, 774–777.
SMITH, G. F. (1970). *Ann. NY Acad. Sci.* **172**, 57–106.
SMITH, G. F. & RIVLIN, R. S. (1958). *Trans. Am. Math. Soc.* **88**, 175–193.
VOIGT, W. (1928). *Lehrbuch der Kristallphysik*. 2. Aufl. Leipzig: Teubner.
WEYL, H. (1946). *The Classical Groups*. New Jersey: Princeton Univ. Press.
WONDRATSCHEK, H. (1952). *Neues Jahrb. Mineral. Monatsh.* **8/9**, 217–234.
WONDRATSCHEK, H. (1953). *Neues Jahrb. Mineral. Monatsh.* **2**, 25–34.
WOOSTER, W. A. (1973). *Tensors and Group Theory for the Physical Properties of Crystals*. Oxford: Clarendon Press.

Acta Cryst. (1980). A**36**, 551–558

Tensor Properties and Rotational Symmetry of Crystals. II. Groups with 1-, 2- and 4-fold Principal Symmetry and Trigonal and Hexagonal Groups Different from Group 3*

BY F. G. FUMI AND C. RIPAMONTI

Istituto di Scienze Fisiche, Universitá di Genova, Italy and GNSM–CNR, Unitá di Genova, Italy

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Abstract

The first part of the paper emphasizes that the problem of the effect of the rotational symmetry of crystals on their tensor properties is completely solved for the groups of 1-, 2- and 4-fold principal symmetry since simple general formulas can be given which provide the schemes of a (polar or axial) general tensor of any rank in these groups, thus yielding a closed-form solution. These formulas are derived both by the new method of vector representatives [introduced in paper I: Fumi & Ripamonti (1980). *Acta Cryst.* A**36**, 535–551] and by the direct-inspection method. In the second part, it is emphasized that simple general rules can be given to obtain the schemes of a (general or particular, polar or axial) tensor of any rank in the trigonal and hexagonal groups other than group 3 from the corresponding scheme in group $3(3_z)$. These rules are given directly by the formulas obtained in the first part for the groups (or generators) of order 2. These compact formulas and rules are applied to two specific tensor properties discussed in recent literature, pointing out errors in some of the reported schemes. Brief discussions are finally given of various techniques to obtain the tensor schemes in the cylindrical and spherical groups, in particular of the new methods introduced in paper I.

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Introduction

In § 2 of paper I (Fumi & Ripamonti, 1980) it was emphasized that the crystallographic groups with 1-, 2- and 4-fold principal symmetry are 'easy groups' for the problem of obtaining the scheme of a tensor, owing to the existence for them of Cartesian orthogonal frames (of the type conventionally adopted in crystal physics) which are purely *permutative* (or *multiplicative*) (Fumi, 1952*a*). The non-vanishing components are at most related to each other in pairs, and the choice of independent components is irrelevant (Fumi, 1952*a*).* Simple, general formulas can thus be given for the schemes of a (polar or axial) general tensor of any rank in these groups (see *e.g.* Jagodzinski & Wondratschek, 1955), thus providing a closed-form solution. In part (*a*) we will use the method of vector representatives introduced in paper I to derive the closed-form solution. We will also see that the solution follows naturally from the direct-inspection method (Fumi, 1952*a*).

In § 2 of paper I it was also emphasized that the trigonal and hexagonal groups other than group $3(3_z)$ are 'very easy groups' for the problem of obtaining the scheme of a tensor, owing to the existence of (conventional) Cartesian orthogonal frames which are purely *multiplicative* for the generators (all of order 2) to be added to the generator 3_z (Fumi, 1952*b*).† The additional relationships between tensor components merely state the vanishing of some components, and the choice of independent components follows from the choice made in group $3(3_z)$ (Fumi, 1952*b*).* Simple, general rules can thus be given for obtaining at once the schemes of a (general or particular, polar or axial) tensor of any rank in these groups from the corresponding scheme in group $3(3_z)$ (see, for example, Jagodzinski & Wondratschek, 1955). In part (*b*) we will present a table of these rules which follows directly from the formulas derived in part (*a*) for the groups (or generators) of order 2.

Part (*a*). Groups with 1-, 2- and 4-fold principal symmetry

(*a*)1. Application of the direct-inspection method

Let us formalize the transformation properties of the (conventional) Cartesian orthogonal tensor components under the generating elements of the groups of interest. We will distinguish simply **g** (*gerade*) *and* **u**(*ungerade*) *tensors*, namely tensors whose components do not change sign, and do change sign, under the inversion, respectively.

We identify the Cartesian orthogonal frame by a set of three orthogonal unit vectors $\hat{\mathbf{i}}$, $\hat{\mathbf{j}}$ and $\hat{\mathbf{k}}$, and we denote by n_i, n_j and n_k the numbers of indices of types i, j and k contained in a given Cartesian orthogonal tensor component.

The generating elements of interest are: the inversion $\bar{1}$, the rotation 2_i of order 2 about the i direction, the rotation–inversion $\bar{2}_i$, the rotation 4_i of order 4 about the i direction, the rotation–inversion $\bar{4}_i$ and the rotation $3_{[111]}$ of order 3 about the direction $\hat{\mathbf{i}}+\hat{\mathbf{j}}+\hat{\mathbf{k}}$.

Let us consider first the generators of order 2. By definition, the inversion $\bar{1}$ multiplies a **g**-tensor component by 1 and a **u**-tensor component by -1. The generators 2_i and $\bar{2}_i$ can be conveniently treated together because their rank-dependent part is only their twofold rotation part. The twofold rotation axis 2_i acts multiplicatively on the coordinates i, j and k through the real multipliers $m_i=+1$, $m_j=m_k=-1$, and thus induces on the tensor components the multiplicative transformation $(-1)^{n_j+n_k}$. The conditions of invariance for the components of a tensor of rank r read then as follows:

for a **g** tensor component under 2_i or $\bar{2}_i$ and for a **u** tensor component under 2_i	$n_j+n_k=$ even, or $n_i=r \bmod 2$;
for a **u** tensor component under $\bar{2}_i$	$n_j+n_k=$ odd, or $n_i=(r+1) \bmod 2$.

Let us consider now the generators 4_i and $3_{[111]}$ for which there is no need to distinguish **g** and **u** tensors. The rotation 4_i sends

$$i\rightarrow i,\quad j\rightarrow k,\quad k\rightarrow -j$$

and thus induces the permutative transformation $(-1)^{n_k}p$, where p permutes j and k, while the rotation $3_{[111]}$ sends

$$i\rightarrow j,\quad j\rightarrow k,\quad k\rightarrow i$$

and thus induces the permutative transformation q, where q permutes i, j and k.

Finally, the transformations induced by the rotation–inversion $\bar{4}_i$ follow at once: for a **g** tensor, they are the same transformations induced by the rotation 4_i, while for a **u** tensor they involve an extra minus sign.

The superposition of the conditions of invariance of the Cartesian orthogonal tensor components under the generating elements of a group yields directly the pertinent closed-form expression of the scheme of a **g** or **u** tensor of any rank. The generating elements adopted for each group are given in Appendix *A* in Table 3.

Table 1 reports the tensor schemes for the various groups. We have used the traditional terminology of 'polar' and 'axial' tensors: **g** tensors include polar

* In these circumstances the new method described in paper I, which involves the use of vector representatives and a criterion for an optimal choice of independent components, reduces obviously to the method of vector representatives.

† The same is true for the generators to be added to the cylindrical axis ∞_z to obtain the groups $\infty 2$, ∞m, ∞/m and ∞/mm.

tensors of even rank and axial tensors of odd rank, while **u** tensors include polar tensors of odd rank and axial tensors of even rank.

(*a*)2. Application of the method of vector representatives

We have shown in paper I (Fumi & Ripamonti, 1980) that the set of numerical coefficients with which a Cartesian orthogonal tensor component enters into a complete family of linearly independent tensor invariants of a group is a valid representative vector of the component when this is subject to the condition of invariance under the group in question.

In the groups of interest here, the permutative (or multiplicative) character of the transformations of the (conventional) Cartesian orthogonal tensor components under the operations of the group ensures the

Table 1. *Schemes for general tensors in the groups with* 1-, 2- *and* 4-*fold principal symmetry*

The groups are designated by the international notation.
The Cartesian orthogonal frames are chosen according to the standard conventions adopted by Nye (1957).
The symbol c denotes a tensor component, and the symbols n_x, n_y and n_z denote its numbers of x, y and z indices.
The symbol r denotes the rank of the tensor.

(*a*) Triclinic, monoclinic and rhombic groups

When it is relevant, the Cartesian orthogonal frame is specified by giving the position of one or two of its axes relative to symmetry elements of the group.

Polar tensors of even rank Axial tensors of odd rank		Polar tensors of odd rank Axial tensors of even rank
All components are independent	$\bar{1}$	All components are zero
Components with $n_y = r$ mod 2 are independent Other components are zero	2 ($y \parallel 2$)	Components as for polar tensors of even rank and axial tensors of odd rank
Components as in 2	m ($y \perp m$)	Components with $n_y = (r+1)$mod 2 are independent Other components are zero
Components as in 2	$2/m$ ($y \parallel 2$)	All components are zero
Components with $n_x = r$ mod 2, $n_y = r$ mod 2 are independent Other components are zero	222 ($x \parallel 2, y \parallel 2$)	Components as for polar tensors of even rank and axial tensors of odd rank
Components as in 222	$mm2$ ($x \perp m, y \perp m$)	Components with $n_x = (r+1)$mod 2, $n_y = (r+1)$mod 2 are independent Other components are zero
Components as in 222	mmm ($x \parallel 2, y \parallel 2$)	All components are zero

(*b*) Tetragonal groups

The z axis of the Cartesian orthogonal frame is parallel to the principal symmetry axis: when this is relevant, the position of the x axis relative to a symmetry element of the group is specified.
The permutation operator p_1 permutes x and y: thus the tensor component p_1c is obtained from c by exchanging its x and y indices.

Polar tensors of even rank Axial tensors of odd rank		Polar tensors of odd rank Axial tensors of even rank
Components with $n_z = r$mod 2 are related as follows: $c = (-1)^{n_x} p_1 c$ Other components are zero	4	Components as for polar tensor of even rank and axial tensors of odd rank
Components as in 4	$\bar{4}$	Components with $n_z = r$mod 2 are related as follows: $c = (-1)^{n_x} p_1 c$ Other components are zero
Components as in 4	$4/m$	All components are zero
Components with $n_x = r$mod 2, $n_y = r$mod 2 are related as follows: $c = (-1)^r p_1 c$ Other components are zero	422 ($x \parallel 2$)	Components as for polar tensor of even rank and axial tensors of odd rank
Components as in 422	$4mm$ ($x \perp m$)	Components with $n_x = (r+1)$mod 2, $n_y = (r+1)$mod 2 are related as follows: $c = -(-1)^r p_1 c$ Other components are zero
Components as in 422	$\bar{4}2m$ ($x \parallel 2$)	Components with $n_x = r$mod 2, $n_y = r$mod 2 are related as follows: $c = -(-1)^r p_1 c$ Other components are zero
Components as in 422	$4/mmm$ ($x \parallel 2$)	All components are zero

Table 1 (*cont.*)

(*c*) Cubic groups

The x, y and z axes of the Cartesian orthogonal frame are parallel to the three symmetry axes of order 2 in the first two groups, and to the three symmetry axes of order 4 in the last three groups.
The permutation operators p_1, p_2 and p_3 permute x, y and z in pairs, while the permutation operators q_1 and q_2 permute x, y and z cyclically. Thus the tensor components p_1c, p_2c and p_3c are obtained from c by exchanging in it the x and y indices, the y and z indices and the z and x indices, respectively. Instead the tensor components q_1c and q_2c are obtained from c by permuting cyclically x with y, y with z, z with x and x with z, z with y, y with x, respectively.

Polar tensors of even rank Axial tensors of odd rank		Polar tensors of odd rank Axial tensors of even rank
Components with $n_x = r\bmod 2$, $n_y = r\bmod 2$ are related as follows: $c = q_1c = q_2c$ Other components are zero	23	Components as for polar tensors of even rank and axial tensors of odd rank
Components as in 23	$m3$	All components are zero
Components with $n_x = r\bmod 2$, $n_y = r\bmod 2$ are related as follows: $c = q_1c = q_2c = (-1)^r p_1c = (-1)^r p_2c = (-1)^r p_3c$ Other components are zero	432	Components as for polar tensors of even rank and axial tensors of odd rank
Components as in 432	$\bar{4}3m$	Components with $n_x = r\bmod 2$, $n_y = r\bmod 2$ are related as follows: $c = q_1c = q_2c = -(-1)^r p_1c = -(-1)^r p_2c = -(-1)^r p_3c$ Other components are zero
Components as in 432	$m3m$	All components are zero

existence of complete sets of independent tensor invariants which are actually *disjoint* (*i.e.* which have *no* components in common). These disjoint tensor invariants are reported in Appendix *A* (Table 3), in a form valid for a **g** or **u** tensor of any rank.

Naturally, the corresponding representative vectors of the Cartesian orthogonal tensor components are particularly simple: since a component enters at most in one invariant, the representative vectors have at most one non-zero entry. Thus, the tensor scheme of a **g** or **u** tensor of any rank in one of these groups follows quite easily. Indeed one can make at once the following statements:

(*a*) components not entering in the disjoint invariants are zero since their representative vectors are zero;

(*b*) components entering in the disjoint invariants are non-zero, since their representative vectors have one non-zero entry.

Furthermore:

(*b*′) components not entering in the same disjoint invariant are unrelated, since their representative vectors are independent owing to the non-correspondence of their non-zero entries;

(*b*″) components entering in the same disjoint invariant are equal when taken with their respective coefficients, since their representative vectors are multiples of each other owing to the correspondence of their non-zero entries.

The closed-form expressions of the tensor schemes read out of the disjoint tensor invariants given in Table 3 are reported in Table 1. It should be mentioned that these results could be obtained by the method of vector representatives also by alternative routes, in which, for example, the method as such would be applied separately to one-generator subgroups of the groups with more than one generator, rather than to the group as a whole, and the results would then be superimposed.

(*a*)3. Schemes for general tensors in the groups with 1-, 2- and 4-fold principal symmetry

The tensor schemes for the groups in question reported in Table 1 are more explicit than those given by Jagodzinski & Wondratschek (1955, Table 8), and are expressed in more compact forms, involving the rank of the tensor. It may be noted that Jagodzinski & Wondratschek obtained their schemes essentially through a formalization of the results given by the direct-inspection method (Fumi, 1952*a*; see Jagodzinski & Wondratschek, 1955, Table 7).

The tensor schemes have a particularly simple character in the triclinic, monoclinic and rhombic groups (Table 1*a*): in these groups, the (conventional) Cartesian orthogonal tensor components undergo purely multiplicative transformations under the operations of the group, and thus the scheme consists simply in identifying the tensor components which are non-zero. In the tetragonal and cubic groups, the tensor schemes have a slightly less simple form (Table 1*b* and *c*). In fact, in these groups the (conventional) Cartesian orthogonal tensor components undergo permutative (or multiplicative) transformations under the operations of the group. Thus the scheme consists in identifying first the tensor components which are non-zero in the subgroup of the given group in which the transformations of the tensor components are purely multiplicative ('multiplicative' subgroup); and in writing then the relations among these tensor components due to the other operations of the group.*

Table 1(*b*) and (*c*) reveals several instances in which the vanishing of a particular tensor component in a given group is not caused by the 'selection rule' due to the 'multiplicative' subgroup of the group, but arises instead from the relations between the tensor components which are non-zero in this subgroup. Specific instances of this type are as follows: the component $n_z = r$ of a **u** tensor in group $\bar{4}$, the component $n_z = r$ of an axial tensor of even rank in group $\bar{4}2m$, and the components $n_x = r$, $n_y = r$ and $n_z = r$ of an axial tensor of even rank in group $\bar{4}3m$. The essential though partial role of the 'multiplicative' subgroup of a crystallographic group in imposing the vanishing of tensor components is explicitly illustrated by the tensor schemes given in Table 1 (and by the rules reported in Table 2 of part (*b*) of this paper). Lax (1974) has formalized the results given by the direct-inspection method (Fumi, 1952*a*,*b*) for the vanishing of tensor components in the groups of 1-, 2- and 4-fold principal symmetry (and for the additional vanishings of tensor components in passing from group $3(3_z)$ to the other trigonal and hexagonal groups) in the form of a 'theorem of the group of indices' and of a 'theorem of the reversal group of indices' (Lax, 1974; theorems 4.4.1 and 4.4.2). These theorems can be paraphrased as follows: consider a given tensor component; identify the elements of the crystal point group which do not transform the component into another component; if one or more of the elements of this 'group of indices' (or of the larger 'reversal group of indices' when the tensor has internal symmetry) changes the sign of the component the component vanishes.

We illustrate the use of Table 1 by one example. Consider a polar tensor of rank 6, symmetric in the exchange of the first two indices and in the permutation of the remaining four indices, in group $\bar{4}2m$. Table 1(*b*) tells us that the components with $n_x = 6\text{mod } 2$, $n_y = 6\text{mod } 2$ are related as follows, $c = (-1)^6 p_1 c$, while the other components are zero. Since $n_x + n_y + n_z = 6$ and n_x and n_y are even, n_z must also be even. There is thus a total of ten possible sets of values for n_x, n_y and n_z: three sets of type 6,0,0; six sets of type 4,2,0; and the set 2,2,2. The components of these sets are connected by the following relations:

600 and 060 $\quad xxxxxx = yyyyyy$;
006 $\quad zzzzzz$;
420 and 240 $\quad xxxxyy = yyxxyy$
and pertinent permutations, namely
$\quad yyxxxx = xxyyyy$
$\quad xyxxxy = xyxyyy$;
402 and 042 $\quad xxxxzz = yyyyzz$
and pertinent permutations, namely
$\quad zzxxxx = zzyyyy$
$\quad zxxxxz = yzyyyz$;
204 and 024 $\quad xxzzzz = yyzzzz$
and pertinent permutations, namely
$\quad zzxxzz = zzyyzz$
$\quad zxxzzz = yzyzzz$;
222 $\quad xxyyzz = yyxxzz$
and pertinent permutations, namely
$\quad zzxxyy$
$\quad zxxyyz = yzxxyz$
$\quad xyxyzz$.

This scheme agrees with the scheme which follows from the quasipotential $\Phi(\hat{\sigma}, E)$ reported by Perfilova, Sirotin & Sonin (1969);* their Table 1 omits, however, the last three non-zero components.

Part (*b*). Trigonal and hexagonal groups other than group 3

The brief discussion of the trigonal and hexagonal groups other than group 3 given in the *Introduction* makes it clear that a particularly convenient approach for obtaining the tensor schemes in these groups is an approach by subgroups, starting from the results for group $3(3_z)$.†

The approach can be viewed, alternatively, as a superposition of the results given by the new methods presented in paper I for the subgroups generated by the generators of each group (specifically, the complete method described in paper I for group $3(3_z)$, and the method of vector representatives for the subgroups generated by the additional generators of order 2), or as an application of the direct-inspection method to the results for group $3(3_z)$ in the spirit of Fumi (1952*b*).

The generators that we choose for the various groups – in accordance with the standard crystallographic settings adopted by Nye (1957) – are as follows:

trigonal groups $\quad 3_z(3)$, $3_z\bar{1}(\bar{3})$, $3_z2_x(32)$, $3_z\bar{2}_x(3m)$, $3_z2_x\bar{1}(\bar{3}m)$;

hexagonal groups $\quad 3_z2_z(6)$, $3_z\bar{2}_z(\bar{6})$, $3_z2_z\bar{1}(6/m)$, $3_z2_z2_x(622)$, $3_z2_z\bar{2}_x(6mm)$, $3_z\bar{2}_z\bar{2}_x(\bar{6}m2)$, $3_z2_z2_x\bar{1}(6/mmm)$.

* It should be noted that in the table for a (polar or axial) general tensor of rank 3 in these groups reported by Fieschi (1957) the symbols *a* (axial) and *p* (polar) at the head of the table must be exchanged. This oversight had already been corrected without mention by Birss (1962) (Tables 2*a* and 2*d*).

* The authors surprisingly assert that the application of the direct method of coordinate transformations to this case is 'very troublesome'. In fact, the group $\bar{4}2m$ is one of the groups in which the direct-inspection method (Fumi, 1952*a*) actually yields the tensor schemes by direct inspection, and thus the application of this method to the case at hand is quite simple though unnecessary owing to the availability of the closed-form expression of the tensor schemes.

† An approach by subgroups is convenient also for cylindrical and spherical groups (see Appendix *B*).

For instance, we treat for convenience the sixfold axis as a superposition of a threefold axis and a twofold axis in the same direction, as Wondratschek (1952) has already done.

The resulting set of general rules to pass from a tensor scheme in group $3(3_z)$ to the corresponding tensor schemes in the various trigonal and hexagonal groups are given in Table 2. These rules coincide, in fact, with the general formulas derived in part (*a*) to obtain the schemes of (general) tensors in the crystallographic groups of order 2.

Table 2 is more explicit than the corresponding table by Jagodzinski & Wondratschek (1955) (Table 9),* and the rules are expressed in more compact form, involving the rank of the tensor. It may be noted that Jagodzinski & Wondratschek (1955) obtained their Table 9 essentially by formalizing the results given by the direct-inspection method (Fumi, 1952*a*,*b*; see Jagodzinski & Wondratschek, 1955, Table 7).

An alternative approach to the derivation by the new methods of the schemes for (general) tensors in these groups would entail the application of the complete method described in paper I (which involves the use of vector representatives and a criterion for an optimal choice of independent components) to each group as a whole. This would, of course, require the construction of the tensor invariants appropriate to the various complete groups: these can, however, be obtained rather simply in a closed form [analogous to the one displayed in paper I for the tensor invariants in group $3(3_z)$] by adopting a (complex) permutative reference frame for each complete group (Sirotin, 1961).*

We use now Table 2 to check the schemes for the (non-tensorial) array for fourth-order elasticity in the trigonal and hexagonal groups other than group 3† obtained by Chung & Li (1974) by applying the direct-inspection method to their results for group 3 in the spirit of Fumi (1952*b*). We find that the schemes reported by Chung & Li (1974) in their Table 1, columns *R*I, *H*II and *H*I, are affected by a number of errors. Some of these errors follow, of course, from the errors for group 3 (Laue group *R*II) discussed in paper I: specifically for group 32 (Laue group *R*I) these errors affect the expressions of 1356, 3455, 4456, 4466, 5556 and 5666, while for group 6 (Laue group *H*II) and for group 622 (Laue group *H*I) they affect the expression of 4466. There are, however, additional errors: these concern specifically the expression of

* It should be noted that for groups 32, $3m$ and $\bar{3}m$, Jagodzinski & Wondratschek (1955) do not use the standard crystallographic setting adopted by Nye (1957). This is due to their choice of a *minimal* global set of generators for all the crystallographic groups which excludes the generators 2_x and $\bar{2}_x$.

* This type of approach is applicable also to the cylindrical groups different from group ∞.

† Fourth-order elasticity is also discussed in Appendix *C* for the case of an isotropic body.

Table 2. *Rules to obtain the schemes of (general or particular) tensors in the various trigonal and hexagonal groups from the scheme for group* 3 (3_z)

The groups are designated by the international notation.
The Cartesian orthogonal frames are chosen according to the standard conventions adopted by Nye (1957). The z axis is parallel to the principal symmetry axis: when this is relevant, the position of the x axis relative to a symmetry element of the group is specified.
The symbols n_x, n_y and n_z denote the numbers of x, y and z indices in a tensor component, while r is the rank of the tensor.

Polar tensors of even rank Axial tensors of odd rank		Polar tensors of odd rank Axial tensors of even rank
Components as in 3	$\bar{3}$	All components are zero
Components with $n_x = r \bmod 2$ as in 3 Other components are zero	32 ($x \parallel 2$)	Components as for polar tensors of even rank and axial tensors of odd rank
Components as in 32	$3m$ ($x \perp m$)	Components with $n_x = (r+1) \bmod 2$ as in 3 Other components are zero
Components as in 32	$\bar{3}m$ ($x \parallel 2$)	All components are zero
Components with $n_z = r \bmod 2$ as in 3 Other components are zero	6	Components as for polar tensors of even rank and axial tensors of odd rank
Components as in 6	$\bar{6}$	Components with $n_z = (r+1) \bmod 2$ as in 3 Other components are zero
Components as in 6	$6/m$	All components are zero
Components with $n_x = r \bmod 2$, $n_z = r \bmod 2$ as in 3 Other components are zero	622 ($x \parallel 2$)	Components as for polar tensors of even rank and axial tensors of odd rank
Components as in 622	$6mm$ ($x \perp m$)	Components with $n_x = (r+1) \bmod 2$, $n_z = r \bmod 2$ as in 3 Other components are zero
Components as in 622	$\bar{6}m2$ ($x \perp m$)	Components with $n_x = (r+1) \bmod 2$, $n_z = (r+1) \bmod 2$ as in 3 Other components are zero
Components as in 622	$6/mmm$ ($x \parallel 2$)	All components are zero

1366 in groups 32, 6 and 622 and the vanishing of 2222 in groups 32 and 622, of 2455 in group 32 and of 1666 in group 6.

APPENDIX *A*

Complete sets of disjoint tensor invariants in the groups with 1-, 2- and 4-fold principal symmetry are reported in Table 3 in a form valid for a **g** or **u** tensor of any rank. They can be obtained straightforwardly by applying the standard projection operator for invariants provided by group theory to the (conventional) Cartesian orthogonal components of the tensors in question. More simply, these invariants can be obtained by using an equivalent operator, introduced by Sirotin (1961) (see paper I, § 3*c* and paper II, part *b*).

APPENDIX *B*

A subgroup approach quite analogous to that of part (*b*) is convenient to obtain the tensor schemes in the cylindrical groups $\infty 2$, ∞m, ∞/m and ∞/mm, starting from the results for group $\infty(\infty_z)$.

Similarly, a convenient treatment of the spherical groups $O^+(3)$ [and $O(3)$] starts from the results for group $\infty(\infty_z)$ and superimposes on these the results for the subgroups generated by the threefold axis $3_{[111]}$ (and by the inversion $\bar{1}$).

Other convenient subgroup treatments of the cylindrical and spherical groups are based on an important theorem by Hermann (1934) which states that tensors of rank $r < n$ cannot distinguish a symmetry axis of order n from an axis of cylindrical symmetry [see, for example, Jagodzinski & Wondratschek (1955) p. 53]: in particular for any tensor of rank $r < 12$, the simple trick of superimposing the results for group $3(3_z)$ and for group $4(4_z)$ yields directly the results for group

Table 3. *Disjoint tensor invariants in the groups with 1-, 2- and 4-fold principal symmetry*

The groups are designated by the international notation.
The Cartesian orthogonal frames are chosen according to the standard crystallographic conventions adopted by Nye (1957) and are specified in the various groups by the generators adopted: a symbol 2_x denotes a twofold rotation axis parallel to the x axis.
The tensor-type symbols g and u stand for *gerade* and *ungerade* tensors, *i.e.* for tensors whose components do not change sign, and do change sign, under the inversion, respectively.
The symbol c denotes a tensor component, and the symbols n_x, n_y and n_z denote its numbers of x, y and z indices.
The symbol r denotes the rank of the tensor.

(*a*) Triclinic, monoclinic and rhombic groups

Group *G* (Generators adopted)	Tensor type	Disjoint tensor invariants
$\bar{1}$	g	Each c
$(\bar{1})$	u	No invariant
2 (2_y)	g, u	Each c with $n_y = r \bmod 2$
m	g	Invariants as in 2
$(\bar{2}_y)$	u	Each c with $n_y = (r+1) \bmod 2$
$2/m$	g	Invariants as in 2
$(2_y, \bar{1})$	u	No invariant
222 $(2_x, 2_y)$	g, u	Each c with $n_x = r \bmod 2$, $n_y = r \bmod 2$
$mm2$	g	Invariants as in 222
$(\bar{2}_x, \bar{2}_y)$	u	Each c with $n_x = (r+1) \bmod 2$, $n_y = (r+1) \bmod 2$
mmm	g	Invariants as in 222
$(2_x, 2_y, \bar{1})$	u	No invariant

Table 3. (*cont.*)

(*b*) Tetragonal groups

The permutation operator p_1 permutes x and y.

Group *G* (Generators adopted)	Tensor type	Disjoint tensor invariants
4 (4_z)	g, u	$c + (-1)^{n_x} p_1 c$ for each c with $n_z = r \bmod 2$
$\bar{4}$	g	Invariants as in 4
$(\bar{4}_z)$	u	$c - (-1)^{n_x} p_1 c$ for each c with $n_z = r \bmod 2$
$4/m$	g	Invariants as in 4
$(4_z, \bar{1})$	u	No invariant
422 $(4_z, 2_x)$	g, u	$c + (-1)^r p_1 c$ for each c with $n_x = r \bmod 2$, $n_y = r \bmod 2$
$4mm$	g	Invariants as in 422
$(4_z, \bar{2}_x)$	u	$c - (-1)^r p_1 c$ for each c with $n_x = (r+1) \bmod 2$, $n_y = (r+1) \bmod 2$
$\bar{4}2m$	g	Invariants as in 422
$(\bar{4}_z, 2_x)$	u	$c - (-1)^r p_1 c$ for each c with $n_x = r \bmod 2$, $n_y = r \bmod 2$
$4/mmm$	g	Invariants as in 422
$(4_z, 2_x, \bar{1})$	u	No invariant

(*c*) Cubic groups

The permutation operators p_1, p_2 and p_3 permute x, y and z in pairs, while the permutation operators q_1 and q_2 permute x, y and z cyclically (see Table 1*c*).

Group *G* (Generators adopted)	Tensor type	Disjoint tensor invariants
23 $(2_z, 3_{[111]})$	g, u	$c + q_1 c + q_2 c$ for each c with $n_x = r \bmod 2$, $n_y = r \bmod 2$
$m3$	g	Invariants as in 23
$(2_z, 3_{[111]}, \bar{1})$	u	No invariant
432 $(4_z, 3_{[111]})$	g, u	$c + q_1 c + q_2 c + (-1)^r (p_1 c + p_2 c + p_3 c)$ for each c with $n_x = r \bmod 2$, $n_y = r \bmod 2$
$\bar{4}3m$	g	Invariants as in 432
$(\bar{4}_z, 3_{[111]})$	u	$c + q_1 c + q_2 c - (-1)^r (p_1 c + p_2 c + p_3 c)$ for each c with $n_x = r \bmod 2$, $n_y = r \bmod 2$
$m3m$	g	Invariants as in 432
$(4_z, 3_{[111]}, \bar{1})$	u	No invariant

$\infty(\infty_z)$, while the simple trick of superimposing the results for group $3(3_z)$ and for group 432 (or $m3m$) yields directly the results for group $O^+(3)$ [or $O(3)$]. The analogous trick of superimposing the results for group $6/mmm$ and for group $m3m$ [adopted, for example by Hearmon (1953) without justification] yields directly the results for group $O(3)$ for any tensor of rank $r < 12$. Similarly, the trick (see Nye, 1957, p. 141) of superimposing the results for group $m3m$ and for the group generated by 8_z (a 'difficult' symmetry axis!) yields directly the results for group $O(3)$ for any tensor of rank $r < 8$. [Juretschke (1975), § 13.3, discusses the simple tricks of superimposing the results for group $4(4_z)$ or $6(6_z)$ (or the results for group $m3m$) with the results for the group generated by a 'suitable' rotation about the z axis, but he cannot make precise statements on the order of the symmetry axis required for a tensor of given rank since he ignores Hermann's (1934) theorem.]

The spherical groups $O^+(3)$ and $O(3)$ can be tackled also by a method entirely analogous to the complete method described in paper I for group $3(3_z)$, *i.e.* by the use of vector representatives with a criterion for an optimal choice of independent components. Complete families of tensor invariants can be constructed by the technique of vector products described by Weyl (1946), or by the use of Weyl's (1946) integrity base. The optimal choice of independent components in $O^+(3)$ can be deduced from the optimal choice for $\infty(\infty_z)$ discussed in paper I. The optimal choice in $O(3)$ is the same as in $O^+(3)$ for **g** tensors, while **u** tensors vanish in $O(3)$.

In this context, one should mention also the treatments of the elastic tensors of an isotropic body based on the construction of the most general invariant expression of the elastic energy in terms of the three basic spherical invariants of the strain and of their products (see Love, 1927; Murnaghan, 1951; Nran'yan, 1965).

APPENDIX *C*

Fourth-order elasticity has been studied for the case of an isotropic body by a number of authors (Krishnamurty, 1963; Nran'yan, 1965; Chung & Li, 1974; Juretschke, 1975), using various types of techniques discussed in Appendix *B*. Krishnamurty (1963), Nran'yan (1965) and Chung & Li (1974) treat a (non-tensorial) array for fourth-order elasticity, while Juretschke (1975) treats the fourth-order elastic tensor: the various authors adopt also different independent components. Nran'yan (1965) uses the technique involving the three basic spherical invariants of the strain: the scheme reported is correct except for an unwanted minus sign in the expression $4455 = 2\cdot 4444$. Chung & Li (1974), instead, adopt essentially Hearmon's (1953) trick: unfortunately, they refer incorrectly to the superposition of the results for group 23 and for group $6(6_z)$ [which yields the results for group $O^+(3)$ only for tensors of rank $r < 6$], but they then superimpose correctly the results for group 432 and for group $6(6_z)$ [or $3(3_z)$]. However, the scheme they report in Table 1, column I is affected by a number of errors: specifically, the following expressions should read as follows: $1155 = 2266 = 4\cdot 1111 - 1112$; $1355 = 4\cdot 1111 + 2\cdot 1112 - 2\cdot 1122$; $1456 = 2456 = 3456 = 8\cdot 1111 - 2\cdot 1112 - 4\cdot 1122 + 2\cdot 1123$; $2333 = 1112$; $2355 = 3\cdot 1112 - 1123$. The correct expressions satisfy the equations reported by Krishnamurty (1963). Finally, Juretschke (1975) (problem 13.17) uses the trick of superimposing the results for group $m3m$ with the results for the group generated by a 'suitable' rotation about the z axis, but he does not specify the order of the rotation to be used (and by referring to § 13.5 he unfortunately implies that the rotation might be 8_z, while the superposition of the results for group $m3m$ and group $8(8_z)$ yields the results for $O(3)$ only for tensors of rank $r < 8$). The scheme reported is affected by various errors: in particular, the components $1456 = 2456 = 3456$ are given as zero, the components $1155 = 2266$ *etc.* are given as equal to 1144, the components $1244 = 2355$ *etc.* are expressed in terms of 1144 and 4444 alone, and an incorrect expression is given for the components $1266 = 2344 = 1355$.

References

BIRSS, R. R. (1962). *Proc. Phys. Soc.* **79**, 946–953.
CHUNG, D. L. & LI, Y. (1974). *Acta Cryst.* A**30**, 1–13.
FIESCHI, R. (1957). *Physica*, **24**, 972–976.
FUMI, F. G. (1952*a*). *Acta Cryst.* **5**, 44–48.
FUMI, F. G. (1952*b*). *Acta Cryst.* **5**, 691–694.
FUMI, F. G. & RIPAMONTI, C. (1980). *Acta Cryst.* A**36**, 535–551.
HEARMON, R. F. S. (1953). *Acta Cryst.* **6**, 331–340.
HERMANN, C. (1934). *Z. Kristallogr.* **89**, 32–48.
JAGODZINSKI, H. & WONDRATSCHEK, H. (1955). *Handbuch der Physik*. Vol. VII. 1, pp. 40–59. Berlin: Springer.
JURETSCHKE, H. J. (1975). *Crystal Physics*. Reading, Mass: Addison Wesley.
KRISHNAMURTY, T. S. G. (1963). *Acta Cryst.* **16**, 839–840.
LAX, M. (1974). *Symmetry Principles in Solid State and Molecular Physics*. New York: John Wiley.
LOVE, A. E. H. (1927). *The Mathematical Theory of Elasticity*. 4th ed. Cambridge University Press.
MURNAGHAN, F. D. (1951). *Finite Deformation of an Elastic Solid*. New York: John Wiley.
NRAN'YAN, A. A. (1965). *Sov. Phys. Solid State*, **6**, 1673–1675.
NYE, J. F. (1957). *Physical Properties of Crystals*. Oxford: Clarendon Press.
PERFILOVA, V. E., SIROTIN, YU. I. & SONIN, A. S. (1969). *Sov. Phys. Crystallogr.* **14**, 136–137.
SIROTIN, YU. I. (1961). *Sov. Phys. Dokl.* **5**, 774–777.
WEYL, H. (1946). *The Classical Groups*. New Jersey: Princeton University Press.
WONDRATSCHEK, H. (1952). *Neues Jahrb. Mineral Monatsh.* **8/9**, 217–234.