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Tensor Properties and Rotational Symmetry of Crystals. I. A New Method for Group $3(3_z)$ and Its Application to General Tensors up to Rank 8*

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Abstract

A new method is presented to overcome the cumbersomeness of the existing methods in the derivation and tabulation of the results for general tensors when the elements of the group do not all simply permute coordinates apart from sign; here the method is described for the generator 3,. The method uses a conjectured, optimal choice of independent components (verified up to rank 8) and a new procedure to obtain the expressions of the dependent components. The independent components adopted consist of sets of components related by appropriate permutations of component indices: this choice is suggested by the similarity of transformation properties of these components. The procedure for the determination of the expressions of dependent components is based on the representation of all components by suitable numerical vectors. The procedure allows the exploitation of the restrictions on the general form of the expressions which follow from the optimal choice of independent components. The method is applied to the derivation of the schemes of general tensors up to rank 8 in group $3(3_7)$. The simplification provided by the method is considerable.

The method permits, for instance, the complete determination of the scheme for the 2^8 components with only x and y indices of a general eighth-rank tensor by solving five systems of linear inhomogeneous equations, one 7 by 7, two 6 by 6 (with identical matrices of coefficients), one 5 by 5 and one 3 by 3. Furthermore, and perhaps more importantly, the resulting scheme can be completely represented by ten distinct expressions (and their permutations). Several errors are pointed out in the table of Chung & Li [Acta Cryst. (1974), A**30**, 1–13] for the (non-tensorial) array for fourth-order elasticity in group 3(3,).

1. A synopsis of the existing methods

The field of tensor properties of crystals is probably the oldest chapter of solid-state physics, and thus the history of the methods used to study the effect of the rotational symmetry of crystals on their tensor properties is a long and involved one. Here we will try to focus on the main ideas of these methods.

A broad distinction can be made between *direct* methods and *indirect* methods. The direct methods work with the tensor as such, while the indirect methods work with the cause-effect relationship defining the tensor or with the expression of a thermodynamic potential involving the tensor.

The typical direct method imposes invariance on each tensor component, *i.e.* imposes equality between each tensor component and its transforms under all the symmetry elements of the crystal. The method, first

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proposed conceptually by Hermann (1934), has since been applied by many authors. Significant improvements of the method are as follows (Fumi, 1952a,b):* (i) the effective use of the correspondence between the transformation properties of Cartesian orthogonal tensor components and of coordinate products; (ii) the consideration of only the generating elements of the crystal point groups; and (iii) the use - whenever possible - of a Cartesian orthogonal frame (in accordance with crystallographic convention) in which the generating elements of the group simply permute coordinates aside from sign (permutative Cartesian orthogonal frame). The method with these three improvements is known as 'the direct-inspection method'. Improvements (i) and (iii) were introduced independently by Landau & Lifschitz: they are used, for example, in Landau & Lifschitz (1959, 1960) but were already essentially present in the first Russian edition (1944) of their book Mechanics of Continuous Media (E. Lifschitz, private communication). Improvements (ii) and (iii) have been used also by Schouten (1951, 1954) and by Wondratschek (1952).

In its initial connotation (Fumi, 1952a,b), the name 'direct-inspection method' referred strictly to the method actually using a (conventional) permutative Cartesian orthogonal frame for the generating elements of the group, and thus applicable only to the groups of 1-, 2- and 4-fold principal symmetry, and to the derivation of the results for the various trigonal and hexagonal groups from the results for group $3(3_2)$: in these cases, the method truly yields the scheme of a tensor by *direct inspection*. The method is described in this form by Nye (1957) and Bhagavantam (1966). Recently, however, some authors (e.g. Lax, 1974) have used the name more loosely for the method of imposing invariance on each tensor component when it includes the three improvements described above, in particular the third one only whenever possible. [Several other authors, e.g. Hearmon (1961), Birss (1966), Mason (1966) and Wooster (1973), appear instead to characterize improperly the direct-inspection method merely by the use of the correspondence with the coordinate products - point (i) - since they seem to consider points (ii) and (iii) as integral parts of the (nameless) typical direct method.]

The specific direct method proposed by Hermann (1934) actually has two versions. The method as presented originally treats separately the effect of each (rotation and rotation-reflection) symmetry axis in its (generally complex) principal axes reference frame, and is thus especially cumbersome to apply in the non-commutative crystal point groups. Here we describe

Hermann's method in a simplified form for the case of a cyclic group, specifically $3(3_2)$. In one version of the method, one identifies first by inspection in the (complex) principal axes frame of the threefold axis the tensor components which are invariant (the only nonvanishing components in this frame), and one then expresses through the known coordinate transformation the Cartesian orthogonal tensor components in terms of the identified invariant components, which are viewed as arbitrary parameters. [This simplified description is given also by Jagodzinski & Wondratschek (1955, p. 53)]. In the other version (which Hermann favoured and applied) one identifies, instead, by inspection the vanishing tensor components in the (complex) principal axes frame of the threefold axis, and then expresses these vanishing components in terms of the Cartesian orthogonal components, again through the known coordinate transformation, thus obtaining relations among the Cartesian orthogonal components.

Another direct method, of group-theoretical nature, imposes invariance to (a minimal set of) linear combinations of tensor components which are bases for the non-identical irreducible representations of the crystal point group, *i.e.* imposes that these linear combinations be equal to zero (Fumi 1952c).* It is in fact sufficient to construct the non-invariant linear combinations of the tensor components which appear in the tensor invariants, since these are the only nonvanishing components. A technical trick of Fumi's method of non-invariants consists in constructing tensorial non-invariants of higher ranks by direct products of invariants and non-invariants of lower rank, thus limiting to a minimum the use of projection operators. The method permits one also to treat together in an efficient way a group and its subgroups.[†] An extension of the method to infinite groups has been published recently by Juretschke (1975).[‡] The extension introduces a new trick to reduce ad hoc the number of non-invariants which would have to be constructed in a straightforward application of the method of non-invariants to the rotation group in three dimensions: the trick (which is not presented clearly) consists simply in exploiting first as far as possible the equivalence of all directions in space by the directinspection method.

Typical indirect methods are the original method by

^{*} The first published presentation and application of the three improvements (specifically to the third-order elastic tensor) is actually given in the paper by Fumi (1951), since the paper by Fumi (1952*a*) submitted in December 1950 was published only in January 1952.

^{*} A brief presentation of the basic idea of the method is given by Heine (1960), p. 309. Bhagavantam (1966), however, ignores the existence of the method (see e.g. p. 82).

[†]Sirotin (1960) quotes the paper by Fumi (1952c), together with papers concerning the direct-inspection method, and ignores the method of non-invariants (Fumi, 1952c). It should be stressed that this method does not proceed step-by-step from low crystallographic symmetry upwards (like, for example, the direct-inspection method), but proceeds instead from groups to subgroups, as Sirotin himself (Sirotin, 1960) proposes to do.

[‡] Unfortunately Juretschke (1975) omits to mention the original paper by Fumi (1952c).

Neumann (1885) and its improvement by Voigt (1928). Neumann imposes invariance under each symmetry element to the general cause–effect relationship defining the tensor, *i.e.* imposes identity with the defining relationship written in Cartesian orthogonal frames equivalent by symmetry, thus obtaining relations among tensor components. Voigt improves Neumann's method by using a defining relationship for the tensor in terms of a scalar (typically a thermodynamic potential), *i.e.* a quantity independent from the reference frame.

Group-theoretical versions of these last two methods have been proposed by various authors (Jahn, 1937; Murnaghan, 1951; Smith & Rivlin, 1958; Fano & Racah, 1959; Landau & Lifschitz, 1959, 1960; Callen, 1968; Lax, 1974). In these methods one obtains conditions on the tensor components by comparing the general defining relationship with the most general defining relationship invariant for the point group of the crystal. Group theory ensures that the most general defining relationship consistent with a symmetry group couples only in all possible ways the *irreducible iso*variants^{*} of the two quantities entering the relationship (see Fano & Racah, 1959, ch. 3, pp. 15-16). The problem is thus to find the irreducible variants of the two quantities, and then to couple the irreducible isovariants with independent, arbitrary constants. In the special case in which one of the two quantities is a scalar, the problem reduces to the search of the invariants of the other quantity, and to the coupling of these invariants to the scalar quantity. It is, in fact, always possible to attack the problem in this special form (see Lax, 1974), since one can always use as the defining relationship of a tensor the scalar constructed by summing the products of each Cartesian orthogonal tensor component by the corresponding product of vector (or pseudovector) components.

Most of the specific methods quoted above differ essentially in the particular technique used to construct the most general expression of a thermodynamic potential invariant in a given group. Jahn (1937) obtains the most general expression of the elastic energy, invariant in a given group, by writing this energy as the triple matrix product of the column vector defined by the irreducible variants of the strain tensor, the invariant elastic constants matrix obtained by coupling the irreducible isovariants of the strain tensor, and the row vector defined again by the irreducible variants of the strain tensor. Murnaghan (1951), on the other hand, obtains the most general expression of the elastic energy (of the first, second and third order in the strain), invariant under a symmetry axis, by identifying by inspection the pertinent strain invariants in the (complex) principal axes frame of the symmetry axis. Landau & Lifschitz (1959, 1960) use a similar technique to obtain the most general invariant expression of various thermodynamic potentials in a trigonal or hexagonal group. Smith & Rivlin (1958) (see also Green & Adkins, 1960) identify, instead, for each crystal point group the basic polynomial strain invariants contained in the so-called 'integrity base' (Weyl, 1946): the most general invariant expression of the elastic energy (to any order in the strain) must be a polynomial function of these basic strain invariants. Callen (1968) considers in particular the problem of constructing the most general expression of a thermodynamic potential bilinear in the cause quantity which is invariant in a given group, and he solves it by constructing a complete set of invariants bilinear in the cause quantity through 'scalar' products of the irreducible isovariants of the quantity itself [the same type of technique used by Jahn (1937) for elasticity]. Lax (1974) generalizes somewhat this last approach. He considers specifically the construction of the most general invariant polynomial of degree equal to the rank of the tensor and involving products of components of two tensorial quantities of generally different rank and type (polar or axial). He solves the problem by constructing a complete set of pertinent invariants through 'scalar' products of the irreducible isovariants of the two tensorial quantities of interest. It should finally be noted that Callen (1968) also applies to several tensor properties in several crystal point groups the type of coupling procedure between cause and effect described by Fano & Racah (1959), and used e.g. by Nowick & Heller (1965, §3.2).

Most direct methods, and the indirect methods of Neumann (1885) and Voigt (1928), lead to systems of linear homogeneous equations among the Cartesian orthogonal tensor components. To find the explicit expressions of the dependent components in terms of a set of independent components, one can solve these equations by the Gauss–Jordan elimination method (see Apostol, 1967).* The systems of equations are particularly involved for high-rank tensors in trigonal and hexagonal groups. In fact, the schemes for general tensors in trigonal and hexagonal groups have as yet been worked out only up to rank 6 (by the method of non-invariants) (Fieschi & Fumi, 1953).†‡ The schemes

^{*} We call irreducible isovariants quantities transforming according to the *same* irreducible representation of the group, and not merely according to equivalent representations.

^{*} One can also adopt Cramer's rule but this requires an *a priori* choice of a set of independent components.

[†] Wondratschek (1953) (who uses a convenient mixture of the two versions of Hermann's method) does not report the explicit expressions of the dependent Cartesian orthogonal components of a general sixth (or fourth) rank tensor in group $3(3_z)$, but only a set of independent equations that the components of the tensor must satisfy.

 $[\]ddagger$ Birss (1966) unfortunately implies that the results of Fieschi & Fumi (1953) for trigonal and hexagonal groups were obtained by the typical direct method (which he does not call the direct-inspection method): in fact, he states explicitly on p. 55 that the results of Fumi (1952c) were obtained in this way, and thus ignores completely the method of non-invariants (Fumi, 1952c).

of one particular tensor of high intrinsic symmetry of rank higher than 6 have also been obtained for these groups, the fourth-order elastic tensor by the method of Voigt (Chung & Li, 1974):* however, the reported schemes contain, unfortunately, a number of errors as we will see in detail in this paper (§ 5) and in paper II (part b).

The group-theoretical versions of the indirect methods, and one version of Hermann's method, lead instead to systems of linear expressions for the Cartesian orthogonal tensor components in terms of arbitrary parameters. The version of Hermann's method in question has apparently never been used as such. The other methods have as yet been applied only to simple cases of essentially didactic interest where it is easy to eliminate the parameters by inspection, and to obtain in this way the explicit expressions of the dependent tensor components (*e.g.* Lax, 1974).

2. Approach to the problem and plan of work

A basic distinction to be made in the problem of obtaining the scheme of a tensor in a point group is the distinction between 'easy' point groups (the groups of 1-, 2- and 4-fold principal symmetry) and 'difficult' point groups (the trigonal and hexagonal groups). The triclinic, monoclinic, rhombic, tetragonal and cubic groups are easy groups because they involve only generators for which there exist Cartesian orthogonal frames (of the type conventionally adopted in crystal physics) which are purely *permutative* (i.e. such that the generators merely permute coordinates apart from sign) or purely multiplicative [i.e. such that the generators merely multiply each coordinate by a numerical factor (specifically ± 1) (Fumi, 1952a)]. The trigonal and hexagonal groups are difficult groups because (and only because) they involve a threefold symmetry axis 3_z for which there does not exist a Cartesian orthogonal frame which is merely permutative. The generators to be added to the threefold axis 3_z to obtain the other trigonal and hexagonal groups are again particularly easy, since for them there exist (conventional) Cartesian orthogonal frames which are purely *multiplicative* (Fumi, 1952b).[†] The relevant consequences of these facts are as follows:

(i) in the groups of 1-, 2- and 4-fold principal symmetry the schemes for general tensors are simple,

with the non-vanishing components at most related to each other in pairs, and it is thus easy to give compact formulas which provide the scheme of a (polar or axial) general tensor of any rank, *i.e.* it is easy to solve the problem in closed form: for this, it is actually sufficient to introduce a suitable notation to formalize the results given by the direct-inspection method (*e.g.* Jagodzinski & Wondratschek, 1955);

(ii) the effect of the threefold axis 3_z must, instead, be studied separately rank by rank;

(iii) the additional relationships between the components of a (general or particular, polar or axial) tensor which appear in passing from group $3(3_z)$ to the other trigonal and hexagonal groups state merely that some components vanish, and it is thus quite easy to express these relationships in closed form: one can repeat the statement made in (i) and quote again the same review article.

This paper presents a new method for studying the effect of the generator 3_z on general tensors. The method uses a conjectured, optimal choice of independent components and adopts numerical vectors representing the tensor components to obtain the expressions of the dependent components: the method simplifies both the derivation of the results and, perhaps more importantly in the era of electronic computers. their tabulation. The method, as characterized by its two features, is in fact useful for any symmetry axis (parallel to a coordinate axis) which does not simply permute coordinates apart from sign (*i.e.* for which the choice of independent components is relevant). The effectiveness of the method is illustrated by its application to general tensors up to rank 8 in group $3(3_{2})$, to give for the first time the schemes of general tensors of ranks 7 and 8.

The other crystal point groups are treated in paper II (Fumi & Ripamonti, 1980), using the notion of vector representatives to give compact derivations of the closed-form results discussed in points (i) and (iii) above.

3. A new method for group 3(3,)

This section describes a new method to obtain the relations among the Cartesian orthogonal components of a general tensor which is invariant in group 3 with $z \parallel 3$ following crystallographic convention.

(a) Two main ideas are the basis of the method. The first idea is to represent the components of an invariant tensor by numerical vectors. In fact the components of a tensor which is invariant in a given group lie in a linear space, since linear combinations of invariant tensor components are also invariant. The adoption of representative vectors permits a *direct* search for the expressions of the dependent components in terms of a

^{*} Chung & Li (1974) treat in fact the (non-tensorial) array C_{pqrs} which enters into the fourth-order term of the elastic energy written as $1/4! \sum_{p < q < r < s} C_{pqrs} \eta_p \eta_q \eta_r \eta_s$ (where p ranges from 1 to 6 and η_p is the pth component of the strain tensor). Surprisingly, they include Fumi (1952*a*,c) and Fieschi & Fumi (1953) among the papers in which the schemes of third-order elastic constants were obtained for all crystal classes, while the complete derivation for the third-order elastic tensor was given by Fumi (1951, 1952*d*).

[†] Unfortunately, Lax (1974) asserts that the problem is 'difficult' whenever one has to deal with a threefold or sixfold symmetry element: he is apparently unaware of the paper by Fumi (1952b).

chosen set of independent components. The coefficients in such an expression are determined by the vector equation obtained by replacing in the expression each component by its representative vector.

The second idea is to make a specific choice of independent components, adopting as such sets of components which are closed under permutations of the maximum possible number of coordinate indices. This choice permits one to express the scheme of an invariant tensor by relatively few distinct relations and by their (generally numerous) permutations, and gives relations of simple form.

The first idea by itself can be made the basis of a method of vector representatives, which is complete as such. The second idea, on the other hand, if included in any of the existing methods, would give permutational compactness to the resulting schemes.

The combination of the two ideas yields a particularly powerful method for group $3(3_2)$. In fact, it is sufficient to derive the expression of one component for each family of dependent components which is closed under appropriate permutations of coordinate indices, and the expression involves only linear combinations of independent components which have the same permutational symmetry of the dependent component in the relevant indices. The expressions of the other dependent components follow at once by simple rules.

(b) An obvious simplifying feature of group $3(3_z)$ is the invariance of z. This feature implies that the problem of writing the relations among the Cartesian orthogonal components of a tensor reduces in fact to a two-dimensional problem in x and y.

Another simplifying feature of group $3(3_z)$ is the possibility of decoupling, for each rank in x and y, the n_y even and n_y odd components $(n_y$, number of y indices): this feature has been exploited, for example, by Fumi (1952c), Fieschi & Fumi (1953) and Wondratschek (1953).

The problem to be tackled in group $3(3_z)$ reduces thus, for each rank in x and y, to the derivation of the expressions of the dependent components with n_y even (or n_y odd) in terms of a chosen set of independent components with n_y even (or n_y odd).

(c) Let us specify now how we choose the representative vector of a Cartesian orthogonal component of an invariant tensor.

Consider a complete family of linearly independent tensor invariants of a given group, constructed by appropriate linear combinations of the Cartesian orthogonal components of a tensor. We note that the set of numerical coefficients with which a given component enters into the family of tensor invariants is a valid representative vector of the component when this is subject to the condition of invariance under the group. Indeed these numerical coefficients satisfy the three following conditions: (i) they transform as the Cartesian orthogonal tensor component under the operations of the group (since they are contravariant to the Cartesian orthogonal tensor component);

(ii) they are invariant under the operations of the group (since a tensor invariant has by definition the same form in frames connected by an operation of the group);

(iii) they are equal in number to the dimension of the linear space of the invariant tensor.

In group $3(3_z)$ we need thus complete families of linearly-independent tensor invariants of the various ranks in x and y. We choose complete families which are very simple to construct and which make particularly simple the determination of the representative vectors of the Cartesian orthogonal tensor components. Consider Hermann's (1934) base for the threefold axis 3_z :

$$x + = x + iy, - = x - iy, z.$$
 (1)

This is a *multiplicative* base (see § 2), since it is the principal axes frame for the threefold axis: in this base, the threefold axis is represented by a 3×3 diagonal matrix with diagonal elements $\exp(2\pi i/3)$, $\exp(-2\pi i/3)$ and 1. Therefore, in this base the construction of tensor invariants of any rank in x and y reduces purely to an inspection, which can be formalized by the compact formula [Hermann, 1934; Wondratschek, 1952; see also Murnaghan (1951) and Landau & Lifshitz (1959, 1960)]*

$$n_+ = n_- \mod 3 \tag{2}$$

(with $n_+ + n_- = \operatorname{rank} \operatorname{in} x$ and y), where n_+ and n_- are the numbers of + and - indices, respectively.[†] Note that a complete family of these tensor invariants of given rank in x and y contains always pairs of complex-conjugate tensor invariants.

Complete families of linearly independent tensor invariants of any given rank in x and y for n_y even and for n_y odd are given by the real parts (Re) and by the imaginary parts (Im) (multiplied by *i*, for convenience) of the tensor invariants provided by (2).[‡] These are the

^{*} Sirotin (1961) rederives (2) in a different context. In fact, he presents a powerful technique for constructing tensor invariants in all the crystallographic groups, which is based on the introduction of a (much) simplified projection operator: the technique has been applied, for example, by Smith (1970).

[†] The corresponding compact formula for group ∞ (∞_z) reads $n_+ = n_-$.

[‡] The splitting of the tensor components of a given rank in x and y into the two sets with n_y even and n_y odd (see § 3b) is easily understood in terms of representative vectors. In fact the elements of the representative vector of a tensor component with n_y even taken from a pair of complex-conjugate tensor invariants given by (2) are equal, while the corresponding elements of the representative vector of a tensor component with n_y odd are equal in absolute value but opposite in sign. This implies that the representative vectors of a component with n_y even and of a component with n_y odd are independent vectors in the linear space of an invariant tensor in x and y. In other words, this linear space splits into two independent linear spaces, one for n_y even and one for n_y odd.

tensor invariants that we use to obtain the representative vectors. To fix the sign of the Im-type invariants, we adopt the convention of taking with a plus sign, in an Im invariant, the monomial invariant in + and - with an even number, n_- , of - symbols on all indices for odd rank, and on all indices but the last for even rank. (The reason for this specific choice will appear clear in the following sections and in the Appendix.) For consistency, we denote then both the Re- and Im-type invariants by this monomial invariant.

The determination of the representative vectors of the Cartesian orthogonal tensor components with n_y even (or with n_y odd) from the pertinent Re-type (or Im-type) tensor invariants can obviously be done directly from the real (or imaginary) parts of the pertinent monomial tensor invariants in + and -. Consider the components with n_y even of a tensor of rank 4. The pertinent Re-type tensor invariants are Re--++, Re-+-+ and Re+--+: the components xxxx and yyyy have coefficient +1 in all three invariants, while the components xxyy and yyxx have coefficient $i^2 = -1$ in the invariant which has the two as first two indices and coefficient $-i^2 = +1$ in the other two invariants.

It should be stressed that the application of representative vectors to obtain the expression of a dependent component in terms of independent components, does not generally require the use of (complete) representative vectors taken from all the pertinent Re- (or Im-) type tensor invariants: it is, in fact, generally sufficient to use 'reduced' representative vectors taken from a few appropriate linear combinations of these tensor invariants (see § 3*e*). This significant simplification is due to the optimal choice of independent components discussed in the next subsection.

(d) The complete families of tensor invariants of the Re (or Im) type of a given rank are closed under

permutations of all indices for odd rank,* while they are closed under permutations of all indices but the last for even rank. The reason for this is easily understood. Each set of monomial invariants in + and - of given rank with given values of n_{\perp} and n_{\perp} provided by (2) is permutationally closed on all indices for any rank. For odd ranks, the construction of the Re- and Im-type invariants does not reduce this permutational closure since the pairs of complex-conjugate monomial invariants belong to different sets of monomial invariants with exchanged values of n_{\perp} and n_{-} . For even ranks, instead, the construction of the Re- and Im-type invariants reduces the permutational closure because the set of monomial invariants with $n_{\perp} = n_{\perp}$ contains within itself the pertinent pairs of complex-conjugate monomial invariants: the reduction in permutational closure is from r to r - 1 indices since the total number of monomial invariants in the set $n_{+} = n_{-}$ is given by r!/(r/2)!(r/2)!, and thus the number of Re- (or Im-) type invariants which can be formed from them is given by 1/2[r!/(r/2)!(r/2)!] = (r - 1)!/(r/2)!(r/2 - 1)!. The Re- and Im-type invariants for even ranks formed from sets of monomial invariants with $n_{\perp} \neq n_{\perp}$ can always be split when necessary into families permutationally closed on r-1 indices. The permutational closure of the Re- and Im-type tensor invariants is illustrated in Table 1 for ranks 2–8. (For rank 1 it is impossible to satisfy (2) and thus there are no tensor invariants in +and -.)

Consider now for each given rank the families of Cartesian orthogonal components with n_y even (or with n_y odd) which have the same permutational symmetry and closure as the pertinent Re- (or Im-) type invariants, on all indices for odd ranks and on all

* In other words, the application of a permutation of indices to an invariant of a family gives always an invariant contained in the family.

 Table 1. Tensor invariants in x and y and corresponding independent Cartesian orthogonal components from rank 2 to rank 8 in group 3 (3.)

	n_y even		n_y odd	
r = 2	Re+ -, 1*	$x \mid x, 1$	i Im + -, 1	$y \mid x, 1$
r = 3	Re + + +, 1	xxx, 1	i Im + + +, 1	<i>yyy</i> , 1
r = 4	$Re(+)+, 3^{\dagger}$	$(yyx)x, 3^{\dagger}$	i Im(+)+, 3	(xxy)x, 3
r = 5	Re(+), 5	(xyyyy), 5	<i>i</i> Im(+), 5	(yxxxx), 5
<i>r</i> = 6	Re(+++)-, 10	(xxxyy)x, 10	i Im(+++-)-, 10	(yyyxx)x, 10
	Re + + + + + +, 1	xxxxx x, 1	i Im + + + + + + + , 1	yyyyy x, 1
<i>r</i> = 7	Re(++++), 21	(xxxxxyy), 21	i Im(+++++-), 21	(yyyyyxx), 21
r = 8	Re(+++)+, 35	(yyyyxxx)x, 35	i Im(++)+, 35	(xxxxyyy)x, 35
	Re(+)-, 7	(yyyyyyx)x, 7	<i>i</i> Im(+)-, 7	(xxxxxxy)x, 7
	Re + + + + + + + + -, 1	xxxxxxx x, 1	i Im + + + + + + + + -, 1	yyyyyyy x, 1

* A vertical dashed line before the last index is used for even ranks when dealing with a single tensor invariant to recall that only the first r-1 indices are permutationally connected.

 \dagger The round bracket indicates how the other tensor invariants (or the other components) of a family can be obtained from the one written out explicitly: it means specifically that one must take the distinct permutations of the + and - indices (or of the x and y indices) inside the bracket. The number next to an invariant (or to a component) gives the number of linearly independent tensor invariants (or of independent components) which can be obtained by this process.

indices but the last for even ranks, the rth index being fixed as x.

These families of Cartesian orthogonal components for ranks 2 to 8 are reported in Table 1 and are valid families of independent components, as will be verified in §§ 4 and 5. We conjecture that the corresponding families of Cartesian orthogonal components for higher ranks will also be valid families of independent components. The existence of sets of independent components formed by permutationally connected components is not surprising owing to the commutation between index permutations and coordinate transformations (Weyl, 1946). The restriction of the permutational connection to r-1 indices in the case of even r can be related to the existence of the set of components with $n_x = n_y$, composed of two subsets linked to each other by the exchange of x with y - acoordinate transformation which does not commute with the operations of the group. We believe this choice of independent components to be optimal both to ease the derivation of the expressions of the dependent components and to give to these expressions a compact form: the pertinent reasons will become apparent in the following sections. The rule for this choice can be formulated as follows, eliminating any direct reference to the Re- and Im-type tensor invariants:

(i) for an odd-rank tensor in x and y, choose as independent Cartesian orthogonal components the components which satisfy the condition $n_x = n_y \mod 3$;*

(ii) for an even-rank tensor in x and y of rank r, choose as independent Cartesian orthogonal components the components which satisfy the condition $n_x = (n_y \pm 1) \mod 6$ on the first r - 1 indices and which have x as last index.[†]

This formulation re-expresses simply in n_x and n_y the conditions on n_+ and n_- which determine the *r* indices of the (monomial) odd-rank tensor invariants, and the first r - 1 indices of the (monomial) even-rank tensor invariants. [Note that the condition $n_+ + n_- = 0 \mod 2$ modifies (2) into $n_+ = n_- \mod 6$, while the condition $n_+ + n_- = 1 \mod 2$ does not modify (2).]‡

(e) We present now the procedure to obtain the expression of a *single* dependent component in terms of the pertinent independent components.

The procedure has two parts. (I) The form of the expression of a given dependent component is dictated by its permutational symmetry in the exchange of indices (due to the repetition of like-coordinate indices), in the sense that the component can depend only on symmetrized linear combinations of the independent components which have the same permutational symmetry on the permutationally connected indices (i.e. all indices for odd-rank tensors and all indices but the last for even-rank tensors). Consider in fact the most general form of the expression of a dependent component in terms of the pertinent independent components. Apply now to both sides of the expression a permutation of indices which exchanges two identical indices of the dependent component in positions corresponding to permutationally connected indices of the independent components: the result is of course a valid expression of the dependent component in terms of the independent components, and its comparison with the initial expression implies equalities among the coefficients of the independent components. (II) The specific values of the coefficients in the expression are easily obtained by replacing the dependent and the independent components by their representative vectors, and by solving the resulting vector equation, *i.e.* the resulting system of linear inhomogeneous equations. In fact (as indicated in I above), one has generally to deal only with the dependent component and with appropriately symmetrized linear combinations of independent components, in a number smaller than the total number of pertinent independent components. It is then sufficient to use a 'reduced' representative vector taken from the (normalized) tensor invariants with the same permutational symmetry as the dependent component on the permutationally connected indices. Indeed, the symmetrized linear combinations of independent components enter only into the linear combinations of the pertinent Re- (or Im-) type tensor invariants which are symmetrized accordingly: this can be seen, for example, from the one-toone correspondence between the elements of the two types of bases of the linear space of the invariant tensor illustrated in Table 1. A simple rule for obtaining the reduced representative vector of a given component is as follows: take as elements of the vector the coefficients with which the component enters into those Re- (or Im-) type tensor invariants which 'correspond' to one (arbitrary) independent component for each symmetrized linear combination of independent components; the 'correspondence' is given by $x \leftrightarrow +, y \leftrightarrow$ for n_y even (and by $y \leftrightarrow +, x \leftrightarrow -$ for n_y odd) on the permutationally connected indices.

A useful tool to simplify calculations, or to effect checks, whenever a given family of independent components is split up in different ways into symmetrized linear combinations in the general forms of the expressions of different dependent components, is given

^{*} The same choice of independent components was adopted for ranks 3 and 5 by Fumi (1952c), Fieschi & Fumi (1953) and Wondratschek (1953), and was proposed by Wondratschek (1953) as a choice for all odd-rank tensors.

[†] For rank 4 the same type of choice of independent components was adopted by Fumi (1952c).

 $[\]pm$ The corresponding rule of group $\infty(\infty_z)$ reads as follows: for an even rank tensor in x and y of rank r, choose as independent Cartesian orthogonal components the components which satisfy the condition $n_x = n_y \pm 1$ on the first r - 1 indices and which have x as last index. [Odd-rank tensors in x and y vanish identically in group $\infty(\infty_z)$.]

by the following rule: the sum of the coefficients with which a given family of independent components enters into a given tensor invariant is (obviously) a fixed number.

Examples of the procedure are given in §4.*

(f) A useful corollary of the procedure described in § 3(e) concerns the connection between the expressions of two dependent components of an even-rank tensor with n_v even which differ one from the other by the exchange of x and y in all indices (e.g. xxxxyy and yyyyxx). The form of the expression of the two components in terms of the independent components is clearly the same. Thus the two systems of linear inhomogeneous equations for the coefficients of the two expressions differ at most in the elements of the representative vectors of the dependent components, and can conveniently be solved together. A specific recipe can also be given for the relation between the representatives of the two dependent components: the representatives taken from the Re-type invariants which satisfy the condition $n_{+} = n_{-} \mod 4$ are equal while those taken from the other Re-type invariants are opposite (see Appendix). This recipe implies that if all the pertinent Re-type invariants satisfy the condition n_{\perp} $= n_{\text{mod}} 4$, the two dependent components are in fact equal.

Of course, the recipe for the relation between the representatives of two components of an even-rank tensor with n_y even differing by the exchange of x and y on all indices is not restricted to the case in which both components are dependent. Thus the recipe can also lead to equality between a dependent and an independent component.

$xxxxxxxxx = c \ \bar{x}\bar{x}\bar{x}\bar{x}\bar{y}\bar{y}\bar{y}\bar{y}x,$

where the symbol $\bar{x}\bar{x}\bar{x}\bar{x}\bar{y}\bar{y}\bar{y}\bar{y}x$ denotes the summation of the 126 independent components (xxxxyyyy)x. It is sufficient to consider the 'reduced' representative vectors of the dependent and of the independent components taken from the Re-type invariant written out explicitly above. The component xxxxxxxxx has clearly representative 1. Sixty-six independent components have also representative 1: they are the component xxxxyyyyx, the (5!/2!3!) (4!/2!2!) = 60 components with two y's in the first five indices (and two y's in the following four indices), and the five components with all four y's in the first five indices. The remaining sixty independent components have, instead, representative -1: they are the 5(4!/3!1!) = 20 components with one y in the first five indices (and three y's in the following four indices) and the (5!/3!2!)4 = 40 components with three y's in the first five indices (and one y in the following four indices). The equation for creads, thus, 1 = c(66 - 60) and c = 1/6.

(g) We present now the procedure to derive directly the explicit expressions of some dependent components from the explicit expressions of other dependent components. This procedure consists of two distinct parts.

The first part concerns the derivation, from the expression of a given dependent component, of the expressions of the other dependent components which can be obtained from the given one by a permutation of the indices corresponding to the permutationally connected indices of the pertinent independent components. The new expressions are obtained immediately from the available expression by applying to both sides of the equality the same permutation on all indices for odd ranks and on all indices but the last for even ranks.*

The second part of the procedure concerns the derivation of the expressions of the dependent components with n_v odd from the expressions of the dependent components with n_v even. For odd-rank tensors, one is dealing with pairs of components, one with n_v even and one with n_v odd, obtained from one another by exchanging x and y in all indices, while for even-rank tensors one is dealing with pairs of components, again one with n_v even and one with n_v odd, obtained from one another by exchanging x and y in all indices but the last. The procedure exploits simply the numerical proportionality between the representative vectors of these pairs of n_{v} - even and n_{v} -odd dependent components of a tensor, and of the analogous pairs of n_y -even and n_v -odd independent components (see § 3d), while keeping in mind that these vectors lie, in fact, in independent linear spaces (see the pertinent footnote in § 3c). This numerical proportionality is established in the Appendix and contains an element of arbitrariness since one is free to multiply, for example, all the representative vectors of the n_v -odd components of a tensor by any numerical factor. For reasons of convenience in the application of the procedure we choose to assert the following:

(i) for odd-rank tensors, the representative vectors of a component with n_y even and of the component with n_y odd obtained from it be exchanging x and y are equal;

(ii) for even-rank tensors, the representative vectors of a component with n_y even and of the component with n_y odd obtained from it by exchanging x and y in the first r - 1 indices are equal or opposite depending on whether the rth index is x or y.

The specific choice of multiplying factor to which these assertions correspond is made clear by the discussion in the Appendix. The rule for obtaining the expressions of the dependent components with n_y odd from the expressions of the dependent components with

^{*} An illustrative example for group $\infty(\infty_r)$ is the following. Consider the x, y components with n_y even of a tensor of rank 10. The pertinent Re-type tensor invariants are Re(+++++----)-, 126 and the pertinent independent components are (xxxxyyyy)x, 126. Consider now specifically the component xxxxxxxxx. The form of its expression in terms of the independent components reads simply

^{*} This type of procedure was adopted also by Fumi (1952c), Fieschi & Fumi (1953) and Wondratschek (1953) in the particular cases in which they chose permutationally closed sets of independent components.

 n_y even thus reads as follows: exchange x and y on both sides of the equality on the permutationally connected indices, with the additional provision of changing the sign of the expression when dealing with a dependent component of an even-rank tensor with n_y even whose last index is y.

Examples of the two procedures are given in § 4.

(h) We have emphasized in § 3(b) that the difficult part of the problem of obtaining the explicit expressions of the dependent components of a tensor in group $3(3_z)$ is the x,y part and we have thus concentrated our discussion on this.

To treat completely a general tensor of rank r, the method is applied in turn to the two families of components of rank r in x and y with n_y even and n_y odd, and to the x,y parts of the two families of components with n_y even and n_y odd of rank r - 1 in x and y, of rank r - 2 in x and y and so on down to rank 1 in x and y.

The expressions of the dependent components of the tensor of total rank r which have a partial rank r' < r in x and y are finally obtained quite simply from the expressions of the x,y parts of these components by putting in (r - r') z indices, and by considering the distinct distributions of the z indices among the x and y indices. Obviously, the component of rank r in z is always an independent component.

4. Examples of application of the new method to general tensors in x and y of ranks 6 and 7 in group 3(3,)

Rank 6

Re-type invariants: Re(+++--)-, 10 and $Re+++++|+, 1^*$

n _y even				n_y odd
xxxxx x	•••••	e‡		<i>ууууу х</i>
ууууу у		0‡	•••••	xxxxx y
(<i>xxxxy</i>)y¶		0 5		(עעעע) ע
(yyyyx)x	•••••	е		(xxxxy)x
(xxxyy)x		e 10	•••••	(<i>yyyxx</i>) <i>x</i>
(yyyxx)y	••••••	0	•••••	(xxxyy)y
		10		

$$yyyyy | y = c_1 \bar{x} \bar{x} \bar{x} \bar{y} \bar{y} | x^{\parallel} + c_2 xxxx | x$$

$$\begin{bmatrix} 1\\-1 \end{bmatrix} = c_1 \begin{bmatrix} 2\\-10 \end{bmatrix} + c_2 \begin{bmatrix} 1\\1 \end{bmatrix}$$

$$yyyyy | y = 1/6 \bar{x} \bar{x} \bar{x} \bar{y} \bar{y} | x + 2/3 xxxx | x$$

$$xxxxx | y = -1/6 \bar{y} \bar{y} \bar{y} \bar{x} | x - 2/3 yyyy | x$$

$$\begin{aligned} xxxxy|y &= c_1 \, \bar{x} \bar{x} \bar{x} \bar{y} y|x + c_2 \, \bar{x} \bar{x} \bar{y} \bar{y} x|x + c_3 \, xxxxx|x \\ \begin{bmatrix} -1 \\ 1 \\ -1 \end{bmatrix} &= c_1 \begin{bmatrix} 2 \\ 0 \\ -4 \end{bmatrix} + c_2 \begin{bmatrix} 0 \\ 2 \\ -6 \end{bmatrix} + c_3 \begin{bmatrix} 1 \\ 1 \\ 1 \end{bmatrix} \\ xxxxy|y &= -1/2 \, \bar{x} \bar{x} \bar{x} \bar{y} y|x + 1/2 \, \bar{x} \bar{x} \bar{y} \bar{y} x|x \\ (xxxy)y &= -1/2 (\bar{x} \bar{x} \bar{x} \bar{y} y)x + 1/2 (\bar{x} \bar{x} \bar{y} \bar{y} \bar{x} x)x \\ (yyyyx)y &= 1/2 (\bar{y} \bar{y} \bar{y} \bar{x} x) x - 1/2 (\bar{y} \bar{y} \bar{x} \bar{x} y)x \end{aligned}$$

$$yyyyx' x = xxxxyy^*$$

$$yyyyx' x = same as for xxxxy'y$$

$$\begin{bmatrix} -1\\1\\1\\1 \end{bmatrix} = same as for xxxxy'y$$

 $yyyyx | x = -2/3 \,\bar{x}\bar{x}\bar{x}\bar{y}y | x + 1/3 \,\bar{x}\bar{x}\bar{y}\bar{y}x | x + 1/3 \,xxxxx | x$ $(yyyyx)x = -2/3(\bar{x}\bar{x}\bar{x}\bar{y}y)x + 1/3(\bar{x}\bar{x}\bar{y}\bar{y}x)x + 1/3 \,xxxxx | x$ $(xxxxy)x = -2/3(\bar{y}\bar{y}\bar{y}\bar{x}x)x + 1/3(\bar{y}\bar{y}\bar{x}\bar{x}y)x + 1/3 \,yyyyy | x$



* The symbol ~ denotes $x \leftrightarrow y$ exchange on all the component indices.

† Short bars *under* indices denote symmetrization on these indices. Thus, $\bar{x}\bar{x}\bar{y}xy$ stands for $xxyxx + xyxxyx + yxxxyx = xxyxyx + xyyxx + \bar{x}yxxyx + xyxxxx + yxxyxx + yxxyxx$.

* The meaning of this round bracket and the role of the vertical dashed line were specified in Table 1.

[†] The rectangular frame encloses the Cartesian orthogonal tensor components which are chosen as independent.

 \ddagger The symbol e (or o) indicates that the representative vectors of the Cartesian orthogonal tensor components on the two sides of the symbol are 'equal' (or 'opposite') (see § 3g).

The symbol 1 indicates that there is only one Cartesian orthogonal tensor component on each side of the symbol e.

¶ The round bracket encloses the indices which are permutationally connected and indicates how one can obtain other independent components from a given independent component, and the expressions of other dependent components from the expression of a given dependent component: specifically it means that one must take the distinct permutations of the x and y indices inside the bracket (with their eventual bars).

|| Short bars *over* indices denote symmetrization on these indices, *i.e.* summation over their distinct permutations: the number placed above the component is the number of distinct permutations.

<i>Rank 7</i> Re-type inva	ariants: Re(+-	++-	++), 21	
n_y even				n_y odd
<i>xxxxxx</i>		1 e	•••••	צעצעצע
(<i>xyyyyyy</i>)		7 e		(yxxxxxx)
(xxxxxyy)		21 e	•••••	(<i>yyyyyxx</i>)
(xxxyyyy)		35 e		(yyyxxxx)
	xxxxxxx	= c	21 XXXXXŸŸ	
	[1]	= c	[-1]	
	xxxxxxx	= -	21 <i>xxxxyy</i>	
	צעצעצע	= -	21 <i>ӯӯӯӯӯҳ</i> ҳ	
		15	6	
xyy	$yyyy = c_1 x \bar{x} \bar{x}$	xxyy	+ $c_2 y \bar{x} \bar{x} \bar{x} \bar{x} \bar{x}$	ÿ
[-	$\begin{bmatrix} 1\\1 \end{bmatrix} = c_1 \begin{bmatrix} -1\\-1 \end{bmatrix}$	1 5]	$+ c_2 \begin{bmatrix} -2\\4 \end{bmatrix}$	
xyy	$yyyy = 1/3 x\bar{x}$	15 x <i>xxy</i>	$\bar{y} + 2/3 y \bar{x} \bar{x} \bar{x} \bar{x}$	κ <u>γ</u>
(<i>xyy</i>	$yyyy) = 1/3(x\bar{x})$	15 XXXŶ	$(\bar{v}) + 2/3(y\bar{x}\bar{x}\bar{x}\bar{x})$	x̄ŷ)
(yxx)	$(xxxx) = 1/3(y\bar{y}\bar{y})$	15 7 7 7 7 7 7 7 7 7 7 7 7 7	$(z) + 2/3(x\bar{y}\bar{y}\bar{y}\bar{y}\bar{y})$	x)

xxxyyyy	$= c_1 x x x \bar{x} \bar{x} \bar{y} \bar{y}$	+ c ₂	12 <i>x̄xӯxxxy</i>	+	$c_3 \bar{x}\bar{y}\bar{y}xxxx$
$\begin{bmatrix} 1\\ -1\\ 1\end{bmatrix}$	$= c_1 \begin{bmatrix} 2\\0\\-6 \end{bmatrix}$	+ c ₂	$\begin{bmatrix} 0\\-2\\4\end{bmatrix}$	+ ($2_3 \begin{bmatrix} -3\\1\\1 \end{bmatrix}$
xxxyyyy	=	1/3	<i>xxyxxxy</i>		1/3 x̄ȳyxxxx
(xxxyyyy)	=	1/3($(\bar{x}\bar{x}\bar{y}xxxy)$	- 1	$\frac{3}{1/3(\bar{x}\bar{y}\bar{y}xxxx)}$
(yyyxxxx)	=	1/30	$(\bar{y}\bar{y}\bar{x}yyyx)$	—	1/3(<i>v̄x̄xyyyy</i>)

5. Tables for general tensors of rank 1 to 8 in group 3(3,)

The complete schemes of general tensors of rank 1 to 8 in group $3(3_z)$ are reported in Table 2.* We give one example of their usage for rank 6. The expression

$$[(xxxyy)z] = -1/3[(\bar{x}\bar{y}\bar{y}yy)z] + 2/3[(yyy\bar{x}\bar{y})z], 60$$

asserts that the explicit expression of the dependent component *xxxyyz* reads

$$xxxyyz = -\frac{1}{3}xyyyz - \frac{1}{3}yxyyz - \frac{1}{3}yyxyz + \frac{2}{3}yyyxz + \frac{2}{3}yyyxz + \frac{2}{3}yyyxz.$$

It asserts also that the expressions of other dependent components can be generated from the expression of xxxyyz by simple permutations of the indices: to obtain the complete set of dependent components of this family one considers the ten distinct permutations of xxxyy and one places z in each of them in the six possible positions. The expression of any one of these dependent components is obtained from the expression of xxxyyz by performing the same permutation on both sides of the equality. For instance, the expression of the dependent component xyzyxx reads

$$xyzyxx = -1/3\bar{x}y\bar{z}y\bar{y}\bar{y} + 2/3y\bar{x}\bar{z}\bar{y}yy$$

We are much indebted to Professor Elliott of the University of Oxford and to Professor Beltrametti of the University of Genoa for many useful discussions. We are also indebted to Professor Elliott for his kind hospitality in the Department of Theoretical Physics at Oxford for brief periods of work and consultation.

APPENDIX

We should note at the onset that the Appendix applies to any axial group with $z \parallel$ axis (and not merely to group 3 with $z \parallel 3$).

We recall first from § 3(c) that the set of numerical coefficients k(C,I) with which a given component C enters into the individual invariants I of a complete family of linearly independent invariants of a given group is a valid representative vector of the component when this is subject to the condition of invariance under the group.

We recall next from § 3(c) that the monomial invariants in + and – are expressed as products of the special coordinates + and – of Hermann's (1934) base.

It follows that the coefficient k(C,I) is the product of the coefficients with which the indices (*i.e.* coordinates x and y) of the component enter into the corresponding indices (*i.e.* special coordinates + and -) of the invariant.

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^{*} The particularization of the results for the tensor of rank 8 to the case of the (non-tensorial) array for fourth-order elasticity treated by Chung & Li (1974) gives the expressions reported in Table 1 of their paper under RII with the exception of the following expressions: $1356 = 2 \cdot 1134 + 3 \cdot 1234$; $3455 = -3 \cdot 3444$; $4456 = \frac{1}{2}(3 \cdot 1444 + 1455)$; $4666 = -2(1115 - 3 \cdot 1125 - 1146)/3$; $5556 = \frac{1}{2}(3 \cdot 1444 + 1455)$; $5666 = 2(1114 - 3 \cdot 1124 + 1156)/3$; and of the expressions for 2455, 2555, 2556 and 4466; the last four expressions are, however, given correctly in the Appendix of their paper. There are also a few cases of errors in the Appendix corrected in Table 1 (*e.g.* the expression for 2266).

Table 2. General tensors of rank 1 to 8 in group $3(z \parallel 3)$

Structure of the table: The table gives the complete schemes of the tensors in a Cartesian orthogonal reference system with $z \parallel 3$, designating the tensor components by their suffixes. It lists the independent components (enclosed in rectangular frames), the expressions of the dependent components in terms of independent components, as well as the components which are zero.

The left-hand part of each rank table includes the components with an even number of y indices, while the right-hand part includes the components with an odd number of y indices.

The horizontal sections of each rank table include components of gradually increasing rank in z.

The dependent components included in a horizontal section of the left-hand part (or of the right-hand part) of each rank table are expressed only in terms of the independent components of the block. Within each block of a rank table, the dependent components are listed in order of decreasing permutational symmetry on all x, y indices for odd rank in x and y, and on all x, y indices but the last for even rank in x and y.

The reader will notice connections between the left-hand and the right-hand parts of each rank table, both in the independent components and in the expressions of the dependent components. Also, the tables of tensors from rank 2 onwards contain horizontal sections derived from the tables for tensors of lower rank. Finally, the compactness of the expressions of the dependent components within each block of a rank table may be noticed. The left-right connections and the compactness of the expressions result from an optimal choice of independent components. The division into horizontal sections arises from the essentially two-dimensional nature of group $3(3_2)$. A more detailed discussion of these points is given in § 3 of the paper.

Notation of the table: The round bracket and the square bracket indicate how one can obtain other independent components from a given independent component, and the expressions of other dependent components from the expression of a given dependent component. The round bracket means that one must take the distinct permutations of the x and y indices inside the bracket (with their eventual bars). The square bracket means that one must take the distinct permutations of the z indices with the x and y indices inside the bracket, subject to the condition that the order of the x and y indices remains unchanged. When a round bracket is enclosed inside a square bracket, subject to the perform first the permutations indicated by the round bracket and then those indicated by the square bracket. The number next to an independent component, or to the expression of a dependent component, gives the total number of independent components or of expressions of dependent components which can be generated by the procedure. Short bars placed over a group of x,y indices denote summation over the distinct permutations of the first group of indices among themselves and of the second group of indices among themselves. The number placed above the component indicates the number of terms in the summation.

Use of the table: An example of the use of the table is given in § 5 of the paper.

The tables for rank 1 to 5 coincide with those reported by Fumi (1952c) and Fieschi & Fumi (1953), but they are more compact. The table for rank 6 differs from the one reported by Fieschi & Fumi (1953) by a better choice of independent components among the components of rank 6 in x and y: the new choice gives more symmetric and more compactable expressions. The tables for rank 7 and rank 8 are entirely new.



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Note now that the exchange of coordinates x and y *induces* an exchange of special coordinates + and -; specifically,

$$\begin{pmatrix} x \\ y \end{pmatrix} \rightarrow \begin{pmatrix} y \\ x \end{pmatrix} \text{ induces } \begin{pmatrix} + \\ - \end{pmatrix} \rightarrow \begin{pmatrix} (i) & - \\ (-i) + \end{pmatrix}.$$

Note also that the coefficient k(C,I) can be written as the product of two coefficients $k(C_a, I_a)k(C_b, I_b)$ where C_a and C_b (and correspondingly I_a and I_b) are products of coordinates x and y (and correspondingly + and -) of lower ranks such that $C = C_a C_b$ (and correspondingly $I = I_a I_b$).

It follows then that the contribution $k(\tilde{C}_a, I_a)$ to the coefficient k(C,I) of a component $C = \tilde{C}_a C_b$, where \tilde{C}_a is the coordinate product exchanged in x and y of the coordinate product C_a , is given by

$$k(\tilde{C}_a, I_a) = m(I_a)k(C_a, \tilde{I}_a),$$

where

$$m(I_a) = i^n (-1)^{n-},$$

with n = (total) number of coordinates in the product C_a (or I_a) and $n_{-} =$ number of - coordinates in the product I_a . \tilde{I}_a is the coordinate product exchanged in + and - of the coordinate product I_a .

none none none [xzzzz] = 0 5 [yzzzz] = 0 zzzzz

(i) Components of odd rank totally exchanged in x and y

Let C be a component even in y, then its representative relative to the invariant $I + \tilde{I}$ is given by

$$k(C, I + \tilde{I}) = k(C, I) + k(C, \tilde{I}).$$

It follows that \tilde{C} has the 'same' representative relative to the invariant $I - \tilde{I}$. Indeed,

$$k(\tilde{C}, I - \tilde{I}) = k(\tilde{C}, I) - k(\tilde{C}, \tilde{I})$$

= $i^{n}(-1)^{n} - k(C, \tilde{I}) - i^{n}(-1)^{\tilde{n}} - k(C, I)$
= $i^{n}[(-1)^{n} - k(C, \tilde{I}) - (-1)^{\tilde{n}} - k(C, I)].$

Since *n* is odd, n_{-} and \tilde{n}_{-} have opposite parity; with the convention of choosing as \tilde{I} the invariants with \tilde{n}_{-} odd (the same convention adopted in § 3*c*), one has

$$k(\tilde{C}, I - \tilde{I}) = i^n [k(C, \tilde{I}) + k(C, I)] = i^n k(C, I + \tilde{I}).$$

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Table 2 (cont.)

Rank 6



 $\{k(C, I + \tilde{I})\}$ are the same, apart from the multiplicative factor in.

(ii) Components of even rank partially exchanged in x and y

Thus the representative vectors $\{k(\tilde{C}, I - \tilde{I})\}$ and $C' \equiv \tilde{C}_a C_x$, which is necessarily odd in y: one has then

$$k(C', I - \overline{I}) = k(C', I) - k(C', I)$$

= $k(\tilde{C}_a, I_a)k(C_x, I_x) - k(\tilde{C}_a, \tilde{I}_a)k(C_x, \tilde{I}_x).$

Let C be a component even in y of the form $C_a C_x$, Since $k(C_x, I_x) = k(C_x, \tilde{I}_x) = 1$, the problem reduces to where C_x is the coordinate x. Consider the component the previous one [point (i)] since the product C_a is of

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Table 2 (cont.)



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Table 2 (cont.)

Rank 8

(<i>yyyyxxx</i>)x, 35 (<i>yyyyyyx</i>)x, 7 <i>xxxxxxxx</i>		(<i>xxx.xyyy</i>) <i>x</i> , 35 (<i>xxxxxxy</i>) <i>x</i> , 7 <i>yyyyyyyx</i>	
$y_{yyyyyyy} = -3/8 \bar{y} \bar{y} \bar{y} \bar{y} \bar{x} \bar{x} \bar{x} - 5/4 \bar{y} \bar{y} \bar{y} \bar{y} \bar{y} \bar{x} x + 27/8 x x x x x x x$		$xxxxxxxy = 3/8 \bar{x} \bar{x} \bar{x} \bar{y} \bar{y} \bar{y} x + 5/4 \bar{x} \bar{x} \bar{x} \bar{x} \bar{x} \bar{y} x - 27/8 yyyyyyyx$	
$(xxxxxxy)y = \frac{1}{24}(\bar{y}\bar{y}\bar{y}\bar{y}\bar{x}\bar{x}x)x - \frac{1}{8}(\bar{y}\bar{y}\bar{y}\bar{x}\bar{x}\bar{x}y)x + \frac{1}{4}(yyyyyyx)x$	7	$(yyyyyyx)y = -\frac{1}{24}(\tilde{x}\tilde{x}\tilde{x}\tilde{x}\tilde{y}\tilde{y}y)x + \frac{1}{8}(\tilde{x}\tilde{x}\tilde{x}\tilde{y}\tilde{y}\tilde{y}x)x - \frac{1}{4}(xxxxxxy)x$	
$-5/12(\bar{y}\bar{y}\bar{y}\bar{y}\bar{y}\bar{y}x)x + 5/8xxxxxxxx$		+ $5/12(\dot{x}\dot{x}\dot{x}\ddot{x}\ddot{x}y)x - 5/8yyyyyyx$	
$(xxxxxyy)x = \frac{1}{3}(\bar{y}\bar{y}\bar{y}\bar{y}\bar{x}xx)x - \frac{1}{3}(\bar{y}\bar{y}\bar{y}\bar{x}xyx)x - \frac{2}{3}(yyyyy\bar{y}\bar{x})x$	21	$(yyyyyxx)x = \frac{1}{3}(\dot{x}\dot{x}\ddot{x}\ddot{y}yy)x - \frac{1}{3}(\dot{x}\ddot{x}\ddot{x}\ddot{y}\dot{y}xy)x - \frac{20}{3}(xxxxx\dot{x}\ddot{x}\ddot{y})x$	
$- \frac{1}{3} (\bar{y} \bar{y} \bar{y} \bar{y} \bar{y} x y y) x + x x x x x x x x x x x x x x x x x $		$- \frac{1}{3}(x \hat{x} \hat{x} \hat{x} \hat{y} x) x + y y y y y y y x$	
$(yyyyyxx)y = 3/8(\bar{y}\bar{y}\bar{y}\bar{y}\bar{x}xx)x - 1/8(\bar{y}\bar{y}\bar{y}\bar{x}\bar{x}yx)x + 3/8(\bar{y}\bar{y}\bar{x}\bar{x}\bar{x}yy)x$	21	$(xxxxxyy)y = -3/8(\bar{x}\bar{x}\bar{x}\bar{x}\bar{y}yy)x + 1/8(\bar{x}\bar{x}\bar{x}\bar{y}\bar{y}\bar{x}y)x - 3/8(\bar{x}\bar{x}\bar{y}\bar{y}\bar{y}\bar{y}xx)x$	
+ $1/4(\bar{y}\bar{y}\bar{y}\bar{y}\bar{y}\bar{y}x)x - 3/8xxxxxxxxx$		$- \frac{1}{4(\tilde{x}\tilde{x}\tilde{x}\tilde{x}\tilde{x}\tilde{y})x} + \frac{3}{8}yyyyyyx}$	
$(xxxxyyy)y = 5/8(yyyxxx)x - 5/24(\tilde{y}\tilde{y}\tilde{y}\tilde{x}yxx)x - 1/24(\tilde{y}\tilde{y}\tilde{x}\tilde{x}yyx)x$	35	(yyyyxxx)y = -5/8(xxxxyyy)x + 5/24(xxxyyy)x + 1/24(xxyyy)x + 1/24(xxyyy)x	
+ $1/8(\bar{y}\bar{x}\bar{x}\dot{x}yy)x + 1/12(yyy)\bar{y}\bar{y}\bar{x})x - 1/4(\bar{y}\bar{y}\dot{y}\dot{x}yy)x$		$- \frac{4}{1/8(\bar{x}\bar{y}\bar{y}\bar{y}xxx)x} - \frac{1}{12(xxx\bar{x}\bar{x}\bar{x}\bar{y})x} + \frac{1}{4(\bar{x}\bar{x}\bar{x}\bar{x}\bar{y}xx)x}$	
+ 3/8 <i>xxxxxxx</i>		– 3/8 <i>yyyyyyx</i>	
[(<i>xxxxxy</i>) <i>z</i>], 168		[(<i>yyyyyxx</i>)z],168	
$[xxxxxxz] = -[\hat{x}\hat{x}\hat{x}\hat{x}\hat{x}\hat{y}\hat{y}z]$	8	$[yyyyyyyz] = -[\hat{y}\hat{y}\hat{y}\hat{y}\hat{x}\hat{x}z]$	
$[(xyyyyyy)z] = \frac{1}{3}[(x\bar{x}\bar{x}\bar{x}\bar{x}\bar{y}\bar{y})z] + \frac{2}{3}[(y\bar{x}\bar{x}\bar{x}\bar{x}\bar{y})z]$	56	$ (vxxxxxx)z = 1/3 (v\tilde{y}\tilde{y}\tilde{y}\tilde{x}\tilde{x})z + 2/3[(x\tilde{y}\tilde{y}\tilde{y}\tilde{y}\tilde{x})z]$	
$[(xxxyyyy)z] = \frac{1}{3}[(\ddot{x}\dot{x}\ddot{y}xxy)z] - \frac{1}{3}[(\ddot{x}\ddot{y}\dot{y}xxx)z]$	280	$[(yyxxxx)z] = \frac{1}{3} [(yyxxxx)z] - \frac{1}{3} [(yxyxx)z] - \frac{3}{3}]$	
(xxxyy)xzz ,280 xxxxxzz ,28		[(<i>yyyxx</i>) <i>xzz</i>],280 [<i>yyyyyxz</i>],28	
$[yyyyyyzz] = 1/6[\bar{x}\bar{x}\bar{x}\bar{y}\bar{y}xzz] + 2/3[xxxxxzz]$	28	$[xxxxxyzz] = -1/6[\tilde{y}\tilde{y}\tilde{y}\tilde{x}\tilde{x}xzz] - 2/3[yyyyyxzz]$	
$[(xxxxy)yzz] = -1/2[(\bar{x}\bar{x}\bar{x}\bar{y}\bar{y})xzz] + 1/2[(\bar{x}\bar{x}\bar{y}\bar{y}x)xzz]$	140	[(yyyyx)yzz] = 1/2[(yyyx)xzz] - 1/2[(yyxx)xzz]]	
$[(yyyyx)xzz] = -2/3[(\bar{x}\bar{x}\bar{x}\bar{y}\bar{y})xzz] + 1/3[(\bar{x}\bar{x}\bar{y}\bar{y}\bar{x})xzz] + 1/3[xxxxxzz]$	140	$[(xxxxy)xzz] = -2/3[(\bar{y}\bar{y}\bar{x}x)xzz] + 1/3[(\bar{y}\bar{y}\bar{x}xy)xzz] + 1/3[yyyyyxzz]$	
[(yyyxx)yzz] = [(xxxyy)xzz] - 1/6[(xxxyy)xzz] + 1/3[xxxxxzz]	280	$[(xxxyy)yzz] = -[(yyyxx)xzz] + 1/6[(\bar{y}\bar{y}\bar{y}\bar{x}\bar{x})xzz] - 1/3[yyyyyxzz]$	
 [(<i>xvvvv</i>)zzz], 280			
[vevvvzzz] = _1/3[\$0000+z=]			
$\left[\left(\frac{2}{2} \right)^{2} - \frac{1}{2} \left(\frac{3}{2} \right)^{2} - \frac{1}{2} \left(\frac{3}{2} \right)^{2} - \frac{1}{2} \left(\frac{2}{2} \right)^{2} - \frac{1}{2} \left(\frac{3}{2} \right)^{2} - \frac{1}{$	56	[yyyyyzzz] = -1/3[yxxxzzz]	
((x,x,y,y),z,z,z) = -1/3((x,y,y,y),z,z,z) + 2/3((y,y,y,y),z,z,z)	560 	$[(yyyxx)zzz] = -1/3[(\tilde{y}\tilde{x}\tilde{x}xx)zzz] + 2/3[(xxx\tilde{y}\tilde{x})zzz]$	
[(<i>yyx</i>) <i>xzzzz</i>],210		[(<i>xxy</i>) <i>xzzzz</i>],210	
$[xxxxzzzz] = [\bar{y}\bar{y}\bar{x}xzzzz]$	70	$[yyyzzzz] = [\hat{x}\hat{x}\hat{y}xzzz]$	
$[yyyyzzzz] = [\bar{y}\bar{y}\bar{x}xzzzz]$	70	$[xxxyzzzz] = -[\tilde{x}\tilde{x}\tilde{y}xzzzz]$	
[(xxy)yzzzz] = [(yyx)xzzzz]	210	[(yyx)yzzzz] = -[(xxy)xzzzz]	

550

Table 2 (cont.)

Rank 8 (cont.) |xxxzzzzz],56 [yyyzzzzz],56 [(xyy)zzzzz] = -[xxxzzzzz]168 [(yxx)zzzzz] = -[yyyzzzzz][xxzzzzzz],28 [yxzzzzzz], 28 [yyzzzzzz] = [xxzzzzzz]28 [xyzzzzz] = -[yxzzzzz]none none [xzzzzzzz] = 08 [vzzzzzzz] = 0

odd rank. It follows that

$$\{k(C', I-\tilde{I})\} = i^n \{k(C, I+\tilde{I})\}.$$

ZZZZZZZZ

Let C now be a component even in y of the form $C_a C_y$. Then for $C' \equiv \tilde{C}_a C_y$, which is necessarily odd in y, one has

$$k(C', I - \tilde{I}) = k(\tilde{C}_a, I_a)k(C_y, I_y) - k(\tilde{C}_a, \tilde{I}_a)k(C_y, \tilde{I}_y),$$

where $k(C_y, \tilde{I}_y) = -k(C_y, I_y) (= \mp i)$. It follows that
 $\{k(C', I - \tilde{I})\} = -i^n \{k(C, I + \tilde{I})\}.$

(iii) Components of even rank totally exchanged in x and y

Let C be a component even in y. Then \tilde{C} is necessarily even in y. One has thus

$$k(\tilde{C}, I+\tilde{I}) = k(\tilde{C}, I) + k(\tilde{C}, \tilde{I})$$
$$= i^n (-1)^{n_-} k(C, \tilde{I}) + i^n (-1)^{\tilde{n}_-} k(C, I).$$

We distinguish two cases for n_{-} and \tilde{n}_{-} :

(a)
$$n_{-}, \tilde{n}_{-}$$
 even; (b) n_{-}, \tilde{n}_{-} odd,

and two cases for n

(A) $n = 0 \mod 4, i^n = +1;$ (B) $n = 2 \mod 4, i^n = -1.$

One has then the following four possibilities:

rank $n = 0 \mod 4$ case (Aa) $k(\tilde{C}, I + \tilde{I}) = k(C, I + \tilde{I});$ case (Ab) $k(\tilde{C}, I + \tilde{I}) = -k(C, I + \tilde{I});$ rank $n = 2 \mod 4$ case (Ba) $k(\tilde{C}, I + \tilde{I}) = -k(C, I + \tilde{I});$ case (Bb) $k(\tilde{C}, I + \tilde{I}) = k(C, I + \tilde{I}).$ These cases can be summarized as follows: for $n_{-} = \tilde{n}_{-} \mod 4$, or equivalently for $n_{-} = n_{+} \mod 4$,

$$k(C) = k(\tilde{C}),$$

otherwise (*i.e.* for $n_{-} \neq \tilde{n}_{-} \mod 4$, or equivalently for $n_{-} \neq n_{+} \mod 4$),

$$k(C) = -k(\tilde{C}).$$

For C and \tilde{C} components odd in y, analogous reasoning leads to the following results:

$$k(C) = -k(\tilde{C}) \quad \text{if } n_{-} = n_{+} \mod 4;$$

$$k(C) = k(\tilde{C}) \quad \text{otherwise.}$$

The results for C and \tilde{C} even in y, and for C and \tilde{C} odd in y, imply that in group 4 (and in the non-crystallographic groups 8, 12 *etc.*) and in group ∞ one has

$$\tilde{C} = C$$
 if C is even in y ($n_y = 0 \mod 2$),
 $\tilde{C} = -C$ if C is odd in y ($n_y = 1 \mod 2$).

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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*

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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. A36, 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 $3(3_2)$. 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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