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**Bao, Gang**

APPLICATION OF GROUP AND INVARIANT-THEORETIC METHODS TO THE  
GENERATION OF CONSTITUTIVE EQUATIONS

*Lehigh University*

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APPLICATION OF GROUP AND INVARIANT-THEORETIC METHODS  
TO THE GENERATION OF CONSTITUTIVE EQUATIONS

by  
Gang Bao

A Dissertation  
Presented to the Graduate Committee  
of Lehigh University  
in Candidacy for the Degree of  
Doctor of Philosophy  
in  
Applied Mathematics

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1987

Approved and recommended for acceptance as a dissertation in  
partial fulfillment of the requirements for the degree of Doctor of  
Philosophy.

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## ABSTRACT

Group representation theory and invariant theory are applied to the generation of constitutive equations. The problem of determining the form of a constitutive expression which is invariant under a group  $G$  is essentially equivalent to the problem of splitting the set of components of the physical tensors appearing in the constitutive expression into sets of quantities which belong to the irreducible representations of the group  $G$ . This approach has been previously employed by Xu, Smith and Smith for crystalline materials and is extended here to include transversely isotropic materials. Product tables for the five transverse isotropy groups are given which should enable one to produce a computer program which will automatically generate constitutive expressions for transversely isotropic materials. The canonical expressions for vector-valued and second-order symmetric tensor-valued form-invariant functions are derived for most of the 32 crystal classes by employing the generating function technique. These analytical results may be used to check the reliability of the existing computer programs due to Xu, Smith and Smith which automatically generate constitutive expressions. Methods which may be employed in determining function bases are discussed and function bases for functions of  $N$  symmetric second-order tensors  $S_1, \dots, S_N$  which are invariant under any given group belonging to the cubic crystal system are given. The concept of irreducibility of a function basis is also discussed.

## 1. Introduction and Mathematical Preliminaries

The theory of group representations and invariant theory play an important role in many branches of mathematics and physics, e.g., in quantum mechanics and in statistics. We are interested in the application of these disciplines to problems arising in continuum mechanics and continuum physics. One of the principal problems is to determine the general form of a constitutive equation

$$T_{i_1 \dots i_n} = G_{i_1 \dots i_n}(E_{p_1 \dots p_m}, \dots) \quad (1.1)$$

which defines the response of a material which possesses symmetry properties. Suppose that the symmetry of a material is specified by a group  $\Gamma$  defined by the set of orthogonal matrices

$$\{\underline{A}\} = \underline{A}_1, \underline{A}_2, \underline{A}_3, \dots \quad (1.2)$$

Then the equations

$$\begin{aligned} & A_{i_1 j_1} \dots A_{i_n j_n} G_{j_1 \dots j_n}(E_{p_1 \dots p_m}, \dots) \\ &= G_{i_1 \dots i_n}(A_{p_1 q_1} \dots A_{p_m q_m} E_{q_1 \dots q_m}, \dots) \end{aligned} \quad (1.3)$$

must hold for each  $\underline{A} = \|[A_{ij}]\|$  belonging to  $\{\underline{A}\}$ . If the functions  $G_{i_1 \dots i_n}$  satisfy (1.3) for all  $\underline{A}$  in  $\{\underline{A}\}$ , we say that (1.3) is invariant under  $\{\underline{A}\}$ . The problem of concern is to determine the canonical form of the functions  $G_{i_1 \dots i_n}$ .

As a simple example, let us consider the constitutive expression for a linear elastic material. The stress-strain law employed in

linear elasticity theory is given by

$$T_{ij} = C_{ijkl} E_{kl} . \quad (1.4)$$

Upon substituting (1.4) into (1.3), we see that the tensor  $C_{ijkl}$  must satisfy the equations

$$C_{ijkl} = A_{ip} A_{jq} A_{kr} A_{ls} C_{pqrs} \quad (1.5)$$

for all  $\underline{A} = ||A_{ij}||$  in  $\{A\}$ . For an isotropic material,  $\{A\}$  is the full orthogonal group. Thus the general expression for  $C_{ijkl}$  is given by

$$C_{ijkl} = \alpha \delta_{ij} \delta_{kl} + \beta \delta_{ik} \delta_{jl} + \gamma \delta_{il} \delta_{jk} . \quad (1.6)$$

Substituting of (1.6) into (1.4) yields the stress-strain law appropriate for an isotropic material.

It may be shown [1] that the problems of determining the form of the polynomial constitutive relation  $\underline{T} = \underline{G}(\underline{E}, \dots)$  appropriate for a material whose symmetry is defined by the group  $\{A\}$  may be reduced to the problem of first determining the form of a scalar-valued polynomial function  $W(\underline{E}, \dots, \underline{T})$  which is invariant under  $\{A\}$ . Thus,  $W$  must satisfy

$$\begin{aligned} & W(E_{i_1 \dots i_m}, \dots, T_{i_1 \dots i_n}) \\ &= W(A_{i_1 j_1} \dots A_{i_m j_m} E_{j_1 \dots j_m}, \dots, A_{i_1 j_1} \dots A_{i_n j_n} T_{j_1 \dots j_n}) \end{aligned} \quad (1.7)$$

for all  $\underline{A}$  belonging to  $\{A\}$ . The problem then is to determine a set of functions  $I_K(\underline{E}, \underline{T}, \dots)$  ( $K=1, \dots, n$ ), each of which is invariant

under  $\{A\}$ , such that any polynomial function  $W(\underline{E}, \underline{F}, \dots)$  invariant under  $\{A\}$  is expressible as a polynomial in the  $I_1, \dots, I_n$ . The invariants  $I_1, \dots, I_n$  are said to form an integrity basis. If one of the elements of such an integrity basis is expressible as a polynomial in the remaining ones, we may, of course, omit it. An integrity basis which is obtained by omitting all such redundant elements is called an irreducible integrity basis.

It is evident that an irreducible integrity basis is not a uniquely determined set of invariants. However, for each degree, the number of invariants needed to form an irreducible integrity basis may be determined by group-theoretical considerations.

It frequently happens that polynomial relations exist between the set of invariants which forms an irreducible integrity basis. Such relations are called syzygies. It follows from the Second Main Theorem of Invariant Theory that all of the syzygies can be derived from a finite number of syzygies. Such a set of syzygies is called a syzygy basis. The existence of syzygies enable us to simplify the general expression of invariants and tensor-valued form-invariant functions.

The polynomial assumption for constitutive equations is not always valid and an alternative method is to find a function basis, i.e., to find a set of invariants such that any invariant is expressible as a single-valued function of them. It can be shown [2] that an integrity basis is also a function basis. However, in general, it will be a reducible function basis. For, although none of the elements  $I_1, \dots, I_n$  of an irreducible integrity basis is expressible as a

polynomial in the remaining ones, one of these may be expressible as a single-valued function in the remaining ones through a syzygy.

The generation of constitutive equations depends, to a large extent, on group representation theory. For a given group  $G$ , a matrix representation

$$\{D\} = D_1, D_2, D_3, \dots$$

of  $G$  is said to be reducible if a matrix  $U$  can be found such that

$$U D_k U^{-1} = \begin{pmatrix} D_k^{(1)} & 0 \\ 0 & D_k^{(2)} \end{pmatrix} \quad (1.8)$$

for all  $k = 1, 2, \dots$ . If there is no  $U$  such that (1.8) holds for all  $D_k \in \{D\}$ , then the representation  $\{D\}$  is said to be irreducible. The irreducible representations of a group may be uniquely determined [3].

The character of a matrix representation  $\{D\}$  is a function on the group  $G$  which is defined by the equation

$$\chi(D_k) = \text{Tr}(D_k), \quad (k=1, 2, \dots) \quad (1.9)$$

The characters of irreducible representations are usually called simple characters. In this thesis, the irreducible representations for a finite group  $G$  are denoted by  $\Gamma_1, \Gamma_2, \dots, \Gamma_n$  and the corresponding simple characters are denoted by  $\chi^{(1)}, \chi^{(2)}, \dots, \chi^{(n)}$ . It can be shown [4] that

$$\frac{1}{g} \sum_{s \in G} \bar{\chi}^{(\mu)}(s) \chi^{(\nu)}(s) = \delta_{\mu\nu} \quad (1.10)$$

holds for any simple characters  $\chi^{(\mu)}$  and  $\chi^{(\nu)}$  of  $G$ . In (1.10),  $g$  is the order of  $G$  and the sum is over all the elements belonging to  $G$ .

Suppose  $\{D\}$  is a reducible representation of  $G$ . Then  $\{D\}$  is expressible as a direct sum of  $\Gamma_1, \Gamma_2, \dots, \Gamma_n$ , i.e.

$$\{D\} = a_1 \Gamma_1 + a_2 \Gamma_2 + \dots + a_n \Gamma_n. \quad (1.11)$$

The number of times the  $\nu^{\text{th}}$  irreducible representation  $\Gamma_\nu$  occurs in  $\{D\}$  is given by

$$a_\nu = \frac{1}{g} \sum_{s \in G} \bar{\chi}^{(\nu)}(s) \chi(s). \quad (1.12)$$

In (1.12),  $\bar{\chi}^{(\nu)}$  is the complex conjugate of  $\chi^{(\nu)}$ ,  $\chi$  is the character of  $\{D\}$  and the sum is over all the elements belonging to  $G$ . The matrices comprising the matrix representation  $\{D\}$  define the manner in which the  $n$  components  $x_1, x_2, \dots, x_n$  of a quantity  $\underline{x}$  transform under the group  $G$ . We may choose  $n$  linearly independent linear combinations  $y_1 = a_{11}x_1 + \dots + a_{1n}x_n, \dots, y_n = a_{n1}x_1 + \dots + a_{nn}x_n$  of the  $x_1, \dots, x_n$  such that the transformation properties of  $(y_1, y_2), (y_3, y_4, y_5), \dots, (y_{n-1}, y_n)$  under the group  $G$  are defined by the irreducible representations  $\Gamma_p, \Gamma_q, \dots, \Gamma_r$  respectively. We then say that  $y = (y_1, y_2)$  is a basic quantity of type  $\Gamma_p$ ,  $\dots, z = (y_{n-1}, y_n)$  is a basic quantity of type  $\Gamma_r$  respectively. This enables us to consider an equivalent invariant-theoretic problem where the algebraic difficulties are substantially reduced. Given a set of quantities  $x_1, x_2, \dots, x_r$

which appear in a constitutive equation, it is important then to obtain all the basic quantities which are linear combinations of  $x_1$ ,  $x_2$ , ...,  $x_r$ .

The work in [5] gives a convenient procedure for generating constitutive expressions for the cases where the symmetry of the material is defined by one of the crystallographic groups. In §2, we extend this work to the case where the symmetry group is one of the five transverse isotropy groups. The results given in §2 should enable us to produce a computer program which will automatically generate constitutive expressions for transversely isotropic materials. In §3, we employ the generating function technique to obtain the general expressions for vector-valued and second-order symmetric tensor-valued functions invariant under one of the 32 crystallographic groups. These analytical results enable us to establish the reliability of the computer programs employed in [5]. In §4, we discuss methods which may be employed in determining function bases for scalar-valued functions  $W(E_1, E_2, \dots, E_n)$  of  $n$  symmetric second-order tensors  $E_1, \dots, E_n$  which are invariant under a given crystallographic group belonging to the cubic crystal system.

The notation employed to denote the various crystallographic groups and a discussion of material symmetry may be found in the books of Hamermesh [3] and Lomont [4].



## 2. Constitutive Relations for Transversely Isotropic Materials

The problem of determining the form of a constitutive expression which is invariant under a group  $G$  is essentially equivalent to the problem of splitting the set of components of the physical tensors appearing in the constitutive expression into sets of quantities which belong to the irreducible representation  $\Gamma_1, \Gamma_2, \dots$  of the group  $G$ . In his doctoral thesis, Xu [6] has employed this idea to develop an intricate computer program which automatically generates constitutive expressions which are invariant under any given crystallographic group. Although the groups considered by Xu are all finite, it will be shown that for continuous groups, such as the transverse isotropy group, the same idea can be employed. In this section, we give the basic information required to extend the results in [6] to the cases where the symmetry group of the material is one of the five transverse isotropy groups which we denote by  $T_1, T_2, \dots, T_5$ . This should enable one to produce a computer program which will automatically generate constitutive expressions for transversely isotropic materials.

In §2.1, we outline a procedure which enables us to conveniently generate the block diagonalized form of matrix constitutive expressions. In §2.2, we give the information required to employ this procedure for the groups  $T_1, T_2, \dots, T_5$ . In §2.3, we give examples of the application of these results to the generation of non-linear constitutive expressions.

## 2.1. Transversely Isotropic Materials

The constitutive expressions which we consider are tensor-valued functions of one or more tensors  $S_1, S_2, \dots$  of degrees  $n_1, n_2, \dots$  in these tensors which are invariant under a group  $\Gamma$  defining the material symmetry. We are primarily interested in the cases where the material symmetry is defined by one of the five groups  $T_1, \dots, T_5$  associated with the various types of transversely isotropic materials. These groups are defined by specifying the groups of  $3 \times 3$  matrices which define the set of equivalent reference frames associated with the material. Thus the group  $T_1$  is comprised of the matrices

$$\underline{Q}(\theta) = \begin{bmatrix} \cos \theta & \sin \theta & 0 \\ -\sin \theta & \cos \theta & 0 \\ 0 & 0 & 1 \end{bmatrix}, \quad 0 \leq \theta < 2\pi. \quad (2.1.1)$$

Let  $\underline{e}_i$  denote the base vectors associated with rectangular Cartesian coordinate system  $x$ . Let  $\bar{\underline{e}}_i$  denote the base vectors associated with the reference frame  $\bar{x}$  which is obtained by rotating the reference frame  $x$  through  $\theta$  radians counter-clockwise. We have

$$\bar{\underline{e}}_i = Q_{ij}(\theta) \underline{e}_j \quad (2.1.2)$$

where the matrix  $\underline{Q}(\theta) = \|Q_{ij}(\theta)\|$  is defined by (2.1.1). If  $x$  and  $\bar{x}$  are equivalent reference frames, i.e. if  $\bar{x}$  arises from  $x$  by applying a symmetry operation to  $x$ , the constitutive equation is required to have the same form when referred to either reference frame. Let  $T_{ij}$  and  $E_{ij}$  denote (absolute) second-order tensors. Then, if

$$T_{ij} = C_{ijkl\dots mn} E_{kl} \dots E_{mn} \quad (2.1.3)$$

is the constitutive expression when referred to the  $x$  frame, the constitutive expression where referred to the  $\bar{x}$  frame is given by

$$\bar{T}_{ij} = \bar{C}_{ijkl\dots mn} \bar{E}_{kl} \dots \bar{E}_{mn} \quad (2.1.4)$$

where

$$\begin{aligned} \bar{T}_{ij} &= Q_{ip} Q_{jq} T_{pq}, \quad \bar{C}_{ij\dots n} = Q_{ip} Q_{jq} \dots Q_{nr} C_{pq\dots r}, \\ \bar{E}_{kl} &= Q_{ks} Q_{lt} E_{st}. \end{aligned} \quad (2.1.5)$$

If the reference frame  $x$  and  $\bar{x}$  are equivalent, we require that

$$\bar{C}_{ijkl\dots mn} = C_{ijkl\dots mn}. \quad (2.1.6)$$

If the symmetry operations consist of all rotations about the  $x_3$  axis, the property tensor  $C_{ijkl\dots mn}$  must satisfy the equations

$$Q_{ip}(\theta) Q_{jq}(\theta) \dots Q_{nu}(\theta) C_{pq\dots u} = C_{ij\dots n} \quad (2.1.7)$$

for  $0 \leq \theta < 2\pi$ . We say that the tensor  $C_{ij\dots n}$  which satisfies (2.1.7) for  $0 \leq \theta < 2\pi$  is invariant under the group  $T_1$ . We may express a tensor which is invariant under the group  $T_1$  as a linear combination of the outer products of the fundamental tensors

$$\sigma_{3i}, \sigma_{1i}\sigma_{1j} + \sigma_{2i}\sigma_{2j} = \alpha_{ij}, \sigma_{1i}\sigma_{2j} - \sigma_{2i}\sigma_{1j} = \beta_{ij} \quad (2.1.8)$$

Thus, one may express the general fourth-order tensor which is invariant under the group  $T_1$  as a linear combination of the

$$\begin{aligned}
& \sigma_{3i}\sigma_{3j}\sigma_{3k}\sigma_{3l},1 ; \quad \alpha_{ij}\alpha_{kl},3 ; \\
& \sigma_{3i}\sigma_{3j}\alpha_{kl},6 ; \quad \alpha_{ij}\beta_{kl},6 ; \\
& \sigma_{3i}\sigma_{3j}\beta_{kl},6 ; \quad \beta_{ij}\beta_{kl},3 ;
\end{aligned} \tag{2.1.9}$$

where the numbers following the tensors denotes the number of distinct isomers of the tensor. An isomer of a tensor  $\sigma_{ijkl}$  is obtained by permuting the subscripts  $i,j,k,l$  of the tensor. We have noted that  $\alpha_{ij} = \alpha_{ji}$  and  $\beta_{ij} = -\beta_{ji}$ . We further note that

$$\beta_{ij}\beta_{kl} = \alpha_{ik}\alpha_{jl} - \alpha_{il}\alpha_{jk} \tag{2.1.10}$$

and that only three of the six isomers of  $\alpha_{ij}\beta_{kl}$  are linearly independent. Thus, we have

$$\begin{aligned}
& \alpha_{ij}\beta_{kl} + \alpha_{ik}\beta_{lj} + \alpha_{il}\beta_{jk} = 0 , \\
& \alpha_{ij}\beta_{kl} + \alpha_{kj}\beta_{li} + \alpha_{lj}\beta_{ik} = 0 , \\
& \alpha_{ik}\beta_{jl} + \alpha_{jk}\beta_{li} + \alpha_{lk}\beta_{ij} = 0 .
\end{aligned} \tag{2.1.11}$$

The existence of relations such as (2.1.11) renders the generation of the general tensor of orders 5,6,... which are invariant under  $T_1$  a non-trivial matter. This may be accomplished using a method [ 7 ] which employs Young tableaux. However the procedure for generating the form of a constitutive equation based on listing the general form of the property tensor  $C_{ijkl\dots mn}$  and then substituting into (2.1.3)

would generally prove to be cumbersome.

It is preferable to employ a procedure based on group representation theory. A set of matrices  $\underline{P}(\theta)$  which is in one to one correspondence with the matrices  $\underline{Q}(\theta)$  comprising the group  $T_1$  and such that  $\underline{P}(\theta_1)\underline{P}(\theta_2)$  corresponds to  $\underline{Q}(\theta_1)\underline{Q}(\theta_2)$  is said to form a matrix representation of the group  $T_1$ . The set of matrices  $K\underline{P}(\theta)K^{-1}$  where  $\det K \neq 0$  also forms a matrix representation of  $T_1$  which is said to be equivalent to the representation  $\underline{P}(\theta)$ . An appropriate choice of the matrix  $K$  enables us to write

$$K\underline{P}(\theta)K^{-1} = \alpha_1 \underline{P}_1(\theta) + \alpha_2 \underline{P}_2(\theta) + \dots \quad (2.1.12)$$

in block diagonal form where  $\alpha_1, \alpha_2, \dots$  are positive integers and where

$$\alpha_1 \underline{P}_1(\theta) + \alpha_2 \underline{P}_2(\theta) = \left\| \begin{array}{ccc} \underline{P}_1(\theta) & \underline{0} & \underline{0} \\ \underline{0} & \underline{P}_1(\theta) & \underline{0} \\ \underline{0} & \underline{0} & \underline{P}_2(\theta) \end{array} \right\| . \quad (2.1.13)$$

We say that the representation  $\underline{P}(\theta)$  may be decomposed into the direct sum of the representations  $\underline{P}_1(\theta), \underline{P}_2(\theta), \dots$ . If a representation  $\underline{P}(\theta)$  cannot be decomposed, it is referred to as an irreducible representation. The irreducible representations associated with  $T_1$  are all one-dimensional and are defined by listing the  $1 \times 1$  matrix corresponding to the matrix  $\underline{Q}(\theta)$ . We define these representations below.

$$\begin{aligned}
\gamma_0 &: 1 \\
\gamma_p &: e^{-ip\theta}, \quad (p=1,2,\dots) \\
\Gamma_p &: e^{ip\theta}, \quad (p=1,2,\dots)
\end{aligned} \tag{2.1.14}$$

$\gamma_0$  denotes the identity representation where the same number 1 corresponds to each  $Q(\theta)$ ;  $\gamma_p$  denote the representation where  $e^{-ip\theta}$  corresponds to  $Q(\theta), \dots$ .

We consider the manner in which a vector transforms under the group  $T_1$ . The components  $\bar{x}_i$  of a vector  $\bar{x}$  when referred to the reference frame  $\bar{x}$  with base vectors  $\bar{e}_i = Q_{ij}(\theta)e_j$  are related to the components  $x_i$  of  $x$  when referred to the  $\bar{x}$  frame with base vectors  $e_i$  by the equations

$$\bar{x}_i = Q_{ij}(\theta)x_j \quad \text{or} \quad \begin{vmatrix} \bar{x}_1 \\ \bar{x}_2 \\ \bar{x}_3 \end{vmatrix} = \begin{vmatrix} \cos\theta & \sin\theta & 0 \\ -\sin\theta & \cos\theta & 0 \\ 0 & 0 & 1 \end{vmatrix} \begin{vmatrix} x_1 \\ x_2 \\ x_3 \end{vmatrix}. \tag{2.1.15}$$

With (2.1.15), we readily see that

$$\begin{vmatrix} \bar{x}_1 + i\bar{x}_2 \\ \bar{x}_1 - i\bar{x}_2 \\ \bar{x}_3 \end{vmatrix} = \begin{vmatrix} e^{-i\theta} & 0 & 0 \\ 0 & e^{i\theta} & 0 \\ 0 & 0 & 1 \end{vmatrix} \begin{vmatrix} x_1 + ix_2 \\ x_1 - ix_2 \\ x_3 \end{vmatrix}. \tag{2.1.16}$$

This tells us that the transformation properties of  $x_1 + ix_2, x_1 - ix_2, x_3$  under the group  $T_1$  are defined respectively by the irreducible

representations  $\gamma_1, \Gamma_1$  and  $\gamma_0$  respectively. We immediately see that the transformation properties of

$$(x_1+ix_2)^2, (x_1+ix_2)(x_1-ix_2), (x_1+ix_2)x_3, (x_1-ix_2)^2, (x_1-ix_2)x_3, x_3^2 \quad (2.1.17)$$

are defined by the irreducible representations  $\gamma_2, \gamma_0, \gamma_1, \Gamma_2, \Gamma_1, \gamma_0$  respectively. Since the components  $x_i x_j$  transform in the same manner as do the components  $S_{ij}$  of a symmetric second-order tensor, we see that the transformation properties of

$$S_{11}-S_{22}+2iS_{12}, S_{11}+S_{22}, S_{13}+iS_{23}, S_{11}-S_{22}-2iS_{12}, S_{13}-iS_{23}, S_{33} \quad (2.1.18)$$

transform according to  $\gamma_2, \gamma_0, \gamma_1, \Gamma_2, \Gamma_1, \gamma_0$  respectively. Similarly we see that

$$\begin{aligned} & (S_{11}-S_{22}+2iS_{12})^2, (S_{11}-S_{22}+2iS_{12})(S_{11}+S_{22}), \\ & (S_{11}-S_{22}+2iS_{12})(S_{13}+iS_{23}), (S_{11}-S_{22}+2iS_{12})(S_{11}-S_{22}-2iS_{12}), \dots \end{aligned} \quad (2.1.19)$$

transform according to  $\gamma_4, \gamma_2, \gamma_3, \gamma_0, \dots$  respectively. Thus, we may readily determine the linear combinations of the components of tensors  $x_i, x_i x_j, x_i x_j x_k, \dots, S_{ij}, S_{ij} S_{kl}, \dots, S_{ij} x_k, S_{ij} x_k x_l, \dots$  which belong to the various irreducible representation  $\gamma_0, \gamma_1, \gamma_2, \dots, \Gamma_1, \Gamma_2, \dots$  of the group  $T_1$ .

Let us consider the problem of determining the linear stress-strain relation for a material whose symmetry is defined by the group

$T_1$  . We write the constitutive expression as

$$\underline{T} = \underline{C}_1 \underline{E}_1 \quad (2.1.20)$$

where

$$\underline{T} = \|t_{11}+t_{22}, t_{33}, t_{11}-t_{22}+2it_{12}, t_{11}-t_{22}-2it_{12}, t_{13}+it_{23}, t_{13}-it_{23}\|^T, \quad (2.1.21)$$

$$\underline{E}_1 = \|e_{11}+e_{22}, e_{33}, e_{11}-e_{22}+2ie_{12}, e_{11}-e_{22}-2ie_{12}, e_{13}+ie_{23}, e_{13}-ie_{23}\|^T$$

and where  $\underline{C}_1$  is a  $6 \times 6$  matrix. If we refer the expression to the reference frame  $\bar{x}$ , whose base vectors are given by  $\bar{e}_i = Q_{ij}(\theta) \underline{e}_j$ , we have

$$\bar{\underline{T}} = \bar{\underline{C}}_1 \bar{\underline{E}}_1, \quad \bar{\underline{T}} = R(\theta) \underline{T}, \quad \bar{\underline{E}}_1 = R(\theta) \underline{E}_1, \quad \bar{\underline{C}}_1 = R(\theta) \underline{C}_1 R^{-1}(\theta) \quad (2.1.22)$$

If the reference frame  $\bar{x}$  is an equivalent reference frame, we require that  $\bar{\underline{C}}_1 = \underline{C}_1$ , i.e.

$$R(\theta) \underline{C}_1 = \underline{C}_1 R(\theta) \quad (2.1.23)$$

we observe from (2.1.14) and (2.1.15) that

$$R(\theta) = \text{diag}(1, 1, e^{-2i\theta}, e^{2i\theta}, e^{-i\theta}, e^{i\theta}) . \quad (2.1.24)$$

With (2.1.23) and (2.1.24), we have 36 equations relating the entries  $C_{ij}(i, j=1, \dots, 6)$  of  $\underline{C}_1$  which are given by



$$c_{11} = c_{11} , c_{12} = c_{12} , c_{13} = e^{-2i\theta} c_{13} , c_{14} = e^{2i\theta} c_{14} , \quad (2.1.25)$$

$$c_{15} = e^{-i\theta} c_{15} , c_{16} = e^{i\theta} c_{16} , \dots$$

with (2.1.25), we have

$$\underline{c}_1 = \begin{pmatrix} c_{11} & c_{12} & 0 & 0 & 0 & 0 \\ c_{21} & c_{22} & 0 & 0 & 0 & 0 \\ 0 & 0 & c_{33} & 0 & 0 & 0 \\ 0 & 0 & 0 & c_{44} & 0 & 0 \\ 0 & 0 & 0 & 0 & c_{55} & 0 \\ 0 & 0 & 0 & 0 & 0 & c_{66} \end{pmatrix} . \quad (2.1.26)$$

This tells us each entry in  $\underline{I}$  which belongs to a representation  $\gamma_p$  is expressible as a linear combination of the elements of  $\underline{E}_1$  which belong to  $\gamma_p$ . Thus, with (2.1.21) and (2.1.26), we see that  $\underline{I} = \underline{c}_1 \underline{E}_1$  may be written as

$$\begin{aligned} \begin{pmatrix} t_{11}+t_{22} \\ t_{33} \end{pmatrix} &= \begin{pmatrix} c_{11}, c_{12} \\ c_{21}, c_{22} \end{pmatrix} \begin{pmatrix} e_{11}+e_{22} \\ e_{33} \end{pmatrix} , \gamma_0 , \\ t_{11}-t_{22}-2it_{12} &= c_{33}(e_{11}-e_{22}+2ie_{12}) , \gamma_2 , \\ t_{11}+t_{22}+2it_{12} &= c_{44}(e_{11}-e_{22}-2ie_{12}) , \gamma_2 , \\ t_{13}+it_{23} &= c_{55}(e_{13}+ie_{23}) , \gamma_1 , \\ t_{13}-it_{23} &= c_{66}(e_{13}-ie_{23}) , \gamma_1 \end{aligned} \quad (2.1.27)$$

where the  $\gamma_0, \dots$  indicates that the quantities in the preceding equation belong to the irreducible representation  $\gamma_0, \dots$ . In (2.1.27), it is clear that we should set  $C_{44} = \bar{C}_{33}$  and  $C_{66} = \bar{C}_{55}$ . If we set  $C_{33} = a + ib$ ,  $C_{55} = c + id$ , the expressions (2.1.27)<sub>3</sub>, ..., (2.1.27)<sub>6</sub> may be written as

$$\begin{pmatrix} t_{11} - t_{22} \\ 2t_{12} \end{pmatrix} = \begin{pmatrix} a, -b \\ b, a \end{pmatrix} \begin{pmatrix} e_{11} - e_{22} \\ 2e_{12} \end{pmatrix}, \quad \begin{pmatrix} t_{13} \\ t_{23} \end{pmatrix} = \begin{pmatrix} c, -d \\ d, c \end{pmatrix} \begin{pmatrix} e_{13} \\ e_{23} \end{pmatrix} \quad (2.1.28)$$

Let us consider the case where the constitutive expression is given by

$$t_{ij} = c_{ijklmn} e_{kl} e_{mn}, \quad t_{ij} = t_{ji}, \quad e_{kl} = e_{lk}. \quad (2.1.29)$$

We write this in matrix form as

$$\underline{T} = \underline{C}_2 \underline{E}_2 \quad (2.1.30)$$

where  $\underline{T}$  is given by (2.1.21) and  $\underline{E}_2$  denotes the  $(21 \times 1)$  column matrix whose entries are linearly independent linear combinations of the 21 quantities  $e_{11}^2, e_{11}e_{12}, \dots$  so chosen that each belongs to one of the irreducible representations of  $T_1$ . With the notation

$$\begin{aligned} E_1 &= e_{11} + e_{22}, \quad E_2 = e_{33}, \quad E_3 = e_{13} + ie_{23}, \quad E_4 = e_{13} - ie_{23}, \\ E_5 &= e_{11} - e_{22} + 2ie_{12}, \quad E_6 = e_{11} - e_{22} - 2ie_{12}, \end{aligned} \quad (2.1.31)$$

we find that the 21 quantities of degree 2 in the  $E_i$  which belong

to  $\gamma_0, \gamma_1, \Gamma_1, \dots$  are given by

$$\begin{aligned} \gamma_0: & E_1^2, E_1 E_2, E_2^2, E_3 E_4, E_5 E_6 ; \\ \gamma_1: & E_1 E_3, E_2 E_3, E_4 E_5 ; & \Gamma_1: & E_1 E_4, E_2 E_4, E_3 E_6 ; \\ \gamma_2: & E_1 E_5, E_2 E_5, E_3^2 ; & \Gamma_2: & E_1 E_6, E_2 E_6, E_4^2 ; & (2.1.32) \\ \gamma_3: & E_3 E_5 ; & \Gamma_3: & E_4 E_6 ; \\ \gamma_4: & E_5^2 ; & \Gamma_4: & E_6^2 . \end{aligned}$$

The constitutive expression  $\underline{T} = \underline{C}_2 \underline{E}_2$  may then be written as

$$\begin{aligned} \left\| \begin{array}{c} t_{11} + t_{22} \\ t_{33} \end{array} \right\| &= \left\| \begin{array}{c} c_1, c_2, c_3, c_4, c_5 \\ c_6, c_7, c_8, c_9, c_{10} \end{array} \right\| \left\| \begin{array}{c} E_1^2 \\ E_1 E_2 \\ E_2^2 \\ E_3 E_4 \\ E_5 E_6 \end{array} \right\|, \gamma_0, \end{aligned} \quad (2.1.33)$$

$$\begin{aligned} t_{13} + it_{23} &= c_{11}E_1E_3 + c_{12}E_2E_3 + c_{13}E_4E_5, \gamma_1, \\ t_{13} - it_{23} &= \bar{c}_{11}E_1E_4 + \bar{c}_{12}E_2E_4 + \bar{c}_{13}E_3E_6, \Gamma_1, \\ t_{11} - t_{22} + 2it_{12} &= c_{14}E_1E_5 + c_{15}E_2E_5 + c_{16}E_3^2, \gamma_2, \\ t_{11} - t_{22} - 2it_{12} &= \bar{c}_{14}E_1E_6 + \bar{c}_{15}E_2E_6 + \bar{c}_{16}E_4^2, \Gamma_2 \end{aligned}$$

where we have noted that  $E_4 = \bar{E}_3$  and  $E_6 = \bar{E}_5$ .

## 2.2. The Irreducible Representations for the Transversely Isotropic Groups

There are five groups which we refer to as transversely isotropic and which are denoted by  $T_1, \dots, T_5$ . These groups are defined by listing matrices such that these matrices or products of these matrices specify all of the symmetry operations associated with the material under consideration. We may refer to these matrices as generators of the group. We then define the irreducible representations associated with a group  $T_i$  by listing the matrices which correspond to the generators of the group.

Suppose that we are given the quantities  $a_1, a_2, \|a_3, a_4\|^T, \|a_5, a_6\|^T, \dots$  belong to the irreducible representations  $\gamma_0, \gamma_1, \gamma_2, \gamma_3, \dots$  of a group and that the quantities  $b_1, b_2, \|b_3, b_4\|^T, \|b_5, b_6\|^T, \dots$  belong to the irreducible representations  $\gamma_0, \gamma_1, \gamma_2, \gamma_3, \dots$  of the same group. We need to determine the linear combinations  $c_i = a_{ijk} a_j b_k$  of the products of the  $a_j$  and  $b_k$  which belong to the various irreducible representations of the group. This information is provided below for the groups  $T_1, \dots, T_5$  in tables which are referred to as product tables. In [5], Xu, Smith and Smith have indicated how these tables may be employed in conjunction with a computer program to automatically generate constitutive expressions. The extension of the results in [5] to include the transversely isotropic materials requires the development of a number of computer programs. This work will be carried out subsequently.

We further list in tables entitled basic quantities the linear combinations of the components of polar vectors  $p_i$ , axial vectors

$a_i$  and symmetric second-order tensors  $S_{ij}$  which belong to the various irreducible representations of the group considered.

(i) The group  $T_1$ .

The group  $T_1$  is comprised of the matrices  $Q(\theta)$  defined by

$$Q(\theta) = \begin{pmatrix} \cos\theta & \sin\theta & 0 \\ -\sin\theta & \cos\theta & 0 \\ 0 & 0 & 1 \end{pmatrix}, \quad 0 \leq \theta < 2\pi. \quad (2.2.1)$$

The group  $T_1$  defines the symmetry of a material which possesses rotational symmetry about the  $x_3$  axis. The irreducible representations associated with the group  $T_1$  are all one dimensional and are given by

$$\begin{aligned} \gamma_0: & 1 \\ \gamma_p: & e^{-ip\theta}, \quad (p=1,2,\dots) \\ \gamma_p: & e^{ip\theta}, \quad (p=1,2,\dots) \end{aligned} \quad (2.2.2)$$

In (2.2.2), the  $1 \times 1$  matrices  $1, e^{-ip\theta}$  and  $e^{ip\theta}$  correspond to the group element  $Q(\theta)$ . The product table is listed below.

Product Table,  $T_1$

$$\begin{aligned}
 \gamma_0: & a_0, b_0; \\
 & a_0 b_0, \\
 & a_p B_p, A_p b_p, (p=1,2,\dots); \\
 \gamma_p: & a_p, b_p; \\
 & a_0 b_p, b_0 a_p, \\
 & a_m b_n, (m,n=1,2,\dots; m+n=p), \\
 & a_m B_n, A_n b_m, (m,n=1,2,\dots; m-n=p); \\
 \Gamma_p: & A_p, B_p; \\
 & a_0 B_p, A_p b_0, \\
 & A_m B_n, (m,n=1,2,\dots; m+n=p), \\
 & A_m b_n, a_n B_m, (m,n=1,2,\dots; m-n=p).
 \end{aligned} \tag{2.2.3}$$

Basic Quantities,  $T_1$

$$\begin{aligned}
 \gamma_0: & p_3, a_3, S_{11}+S_{22}, S_{33} \\
 \gamma_1: & p_1+ip_2, a_1+ia_2, S_{13}+iS_{23} \\
 \Gamma_1: & p_1-ip_2, a_1-ia_2, S_{13}-iS_{23} \\
 \gamma_2: & S_{11}-S_{22}+2iS_{12} \\
 \Gamma_2: & S_{11}-S_{22}-2iS_{12}
 \end{aligned} \tag{2.2.4}$$

(ii) The group  $T_2$

The group  $T_2$  is comprised of the matrices  $\underline{Q}(\theta)$  and  $\underline{R}_1 \underline{Q}(\theta)$  where  $0 \leq \theta < 2\pi$  and where

$$\underline{Q}(\theta) = \begin{pmatrix} \cos\theta & \sin\theta & 0 \\ -\sin\theta & \cos\theta & 0 \\ 0 & 0 & 1 \end{pmatrix}, \quad \underline{R}_1 = \text{diag}(-1, 1, 1). \quad (2.2.5)$$

The irreducible representations associated with the group  $T_2$  are defined by listing the matrices corresponding to the group elements  $\underline{Q}(\theta)$  and  $\underline{R}_1$ . We denote the irreducible representations by

$$\gamma_0: 1, 1$$

$$\Gamma_0: 1, -1$$

$$\gamma_p: \begin{pmatrix} e^{-ip\theta} & 0 \\ 0 & e^{ip\theta} \end{pmatrix}, \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}, \quad (p=1, 2, \dots) \quad (2.2.6)$$

where the first and second matrices correspond to  $\underline{Q}(\theta)$  and  $\underline{R}_1$  respectively. The product table is listed below.

Product Table,  $T_2$

$$\begin{aligned}
 \gamma_0: & a_0, b_0; \\
 & a_0 b_0, A_0 B_0, \\
 & a_{m1} b_{m2} + a_{m2} b_{m1}, (m=1,2,\dots); \\
 \Gamma_0: & A_0, B_0; \\
 & a_0 B_0, A_0 b_0, \\
 & a_{m1} b_{m2} - a_{m2} b_{m1}, (m=1,2,\dots); \quad (2.2.7) \\
 \gamma_p: & \|a_{p1}, a_{p2}\|^T, \|b_{p1}, b_{p2}\|^T; \\
 & \|a_0 b_{p1}, a_0 b_{p2}\|^T, \|a_{p1} b_0, a_{p2} b_0\|^T, \\
 & \|A_0 b_{p1}, -A_0 b_{p2}\|^T, \|a_{p1} B_0, -a_{p2} B_0\|^T, \\
 & \|a_{m1} b_{n1}, a_{m2} b_{n2}\|^T, (m,n=1,2,\dots; m+n=p), \\
 & \|a_{m1} b_{n2}, a_{m2} b_{n1}\|^T, \|a_{n2} b_{m1}, a_{n1} b_{m2}\|^T, (m,n=1,2,\dots; m-n=p).
 \end{aligned}$$

Basic Quantities,  $T_2$

$$\begin{aligned}
 \gamma_0: & p_3, S_{11} + S_{22}, S_{33} \\
 \Gamma_0: & a_3 \\
 \gamma_1: & \|p_1 + ip_2, -p_1 + ip_2\|^T, \|a_1 + ia_2, a_1 - ia_2\|^T, \quad (2.2.8) \\
 & \|S_{13} + iS_{23}, -S_{13} + iS_{23}\|^T \\
 \gamma_2: & \|S_{11} - S_{22} + 2iS_{12}, S_{11} - S_{22} - 2iS_{12}\|^T
 \end{aligned}$$



(iii) The group  $T_3$

The group  $T_3$  is comprised of the matrices  $\underline{Q}(\theta)$  and  $\underline{R}_3 \underline{Q}(\theta)$  where  $0 \leq \theta < 2\pi$  and where

$$\underline{Q}(\theta) = \begin{pmatrix} \cos\theta & \sin\theta & 0 \\ -\sin\theta & \cos\theta & 0 \\ 0 & 0 & 1 \end{pmatrix}, \quad \underline{R}_3 = \text{diag}(1, 1, -1). \quad (2.2.9)$$

The irreducible representations associated with the group  $T_3$  are defined by listing the matrices corresponding to the group elements  $\underline{Q}(\theta)$  and  $\underline{R}_3$ . We denote the irreducible representations by

$$\begin{aligned} \gamma_0 &: 1, 1 \\ \Gamma_0 &: 1, -1 \\ \gamma_p &: e^{-ip\theta}, 1; \quad \bar{\gamma}_p: e^{ip\theta}, 1, \quad (p=1, 2, \dots) \\ \Gamma_p &: e^{-ip\theta}, -1; \quad \bar{\Gamma}_p: e^{ip\theta}, -1, \quad (p=1, 2, \dots) \end{aligned} \quad (2.2.10)$$

where the first and second  $1 \times 1$  matrices correspond to  $\underline{Q}(\theta)$  and  $\underline{R}_3$  respectively. The product table is listed below.

Product Table,  $T_3$

$$\begin{aligned}
 \Upsilon_0: & a_0, b_0; \\
 & a_0 b_0, A_0 B_0, \\
 & a_m \bar{b}_m, \bar{a}_m b_m, A_m \bar{B}_m, \bar{A}_m B_m, (m=1,2,\dots); \\
 \Gamma_0: & A_0, B_0; \\
 & a_0 B_0, A_0 b_0, \\
 & a_m \bar{B}_m, \bar{a}_m B_m, A_m \bar{B}_m, \bar{A}_m b_m, (m=1,2,\dots); \\
 \Upsilon_p: & a_p, b_p; \\
 & a_0 b_p, a_p b_0, A_0 B_p, A_p B_0, \\
 & a_m b_n, A_m B_n, (m,n=1,2,\dots; m+n=p), \\
 & a_m \bar{b}_n, \bar{a}_n b_m, A_m \bar{B}_n, \bar{A}_n B_m, (m,n=1,2,\dots; m-n=p); \\
 \bar{\Upsilon}_p: & \bar{a}_p, \bar{b}_p; \\
 & a_0 \bar{b}_p, \bar{a}_p b_0, A_0 \bar{B}_p, \bar{A}_p B_0, \\
 & \bar{a}_m \bar{b}_n, \bar{A}_m \bar{B}_n, (m,n=1,2,\dots; m+n=p), \\
 & \bar{a}_m b_n, a_n \bar{b}_m, \bar{A}_m B_n, A_n \bar{B}_m, (m,n=1,2,\dots; m-n=p); \\
 \Gamma_p: & A_p, B_p; \\
 & a_0 B_p, A_p b_0, A_0 b_p, a_p B_0, \\
 & a_m B_n, A_m B_n, (m,n=1,2,\dots; m+n=p), \\
 & a_m \bar{B}_n, \bar{a}_n B_m, A_m \bar{b}_n, \bar{A}_n b_m, (m,n=1,2,\dots; m-n=p); \\
 \bar{\Gamma}_p: & \bar{A}_p, \bar{B}_p; \\
 & a_0 \bar{B}_p, \bar{A}_p b_0, A_0 \bar{b}_p, \bar{a}_p B_0, \\
 & \bar{a}_m \bar{B}_n, \bar{A}_m \bar{b}_n, (m,n=1,2,\dots; m+n=p), \\
 & \bar{a}_m B_n, a_n \bar{B}_m, \bar{A}_m b_n, A_n \bar{b}_m, (m,n=1,2,\dots; m-n=p).
 \end{aligned} \tag{2.2.11}$$

Basic Quantities,  $T_3$

$$\begin{aligned}
 \gamma_0: & a_3, S_{11}+S_{22}, S_{33} \\
 \Gamma_0: & p_3 \\
 \gamma_1: & p_1+ip_2 \\
 \bar{\gamma}_1: & p_1-ip_2 \\
 \Gamma_1: & a_1+ia_2, S_{13}+iS_{23} \\
 \bar{\Gamma}_1: & a_1-ia_2, S_{13}-iS_{23} \\
 \gamma_2: & S_{11}-S_{22}+2iS_{12} \\
 \bar{\gamma}_2: & S_{11}-S_{22}-2iS_{12}
 \end{aligned} \tag{2.2.12}$$

(iv) The group  $T_4$

The group  $T_4$  is comprised of the matrices  $Q(\theta), R_1 Q(\theta), R_3 Q(\theta)$  and  $R_1 R_3 Q(\theta)$  where  $0 \leq \theta < 2\pi$  and where

$$Q(\theta) = \begin{pmatrix} \cos\theta & \sin\theta & 0 \\ -\sin\theta & \cos\theta & 0 \\ 0 & 0 & 1 \end{pmatrix}, \quad R_1 = \text{diag}(-1, 1, 1), \quad R_3 = \text{diag}(1, 1, -1) \tag{2.2.13}$$

The irreducible representations associated with the group  $T_4$  are defined by listing the matrices corresponding to the group elements  $Q(\theta)$ ,  $R_1$  and  $R_3$ . We denote the irreducible representations by

$$\gamma_{01}: 1, 1, 1$$

$$\gamma_{02}: 1, 1, -1$$

$$\gamma_{03}: 1, -1, 1$$

$$\gamma_{04}: 1, -1, -1$$

$$\gamma_p: \begin{vmatrix} e^{-ip\theta} & 0 \\ 0 & e^{ip\theta} \end{vmatrix}, \begin{vmatrix} 0 & 1 \\ 1 & 0 \end{vmatrix}, \begin{vmatrix} 1 & 0 \\ 0 & 1 \end{vmatrix}, \quad (p=1,2,\dots) \quad (2.2.14)$$

$$\Gamma_p: \begin{vmatrix} e^{-ip\theta} & 0 \\ 0 & e^{ip\theta} \end{vmatrix}, \begin{vmatrix} 0 & 1 \\ 1 & 0 \end{vmatrix}, \begin{vmatrix} -1 & 0 \\ 0 & -1 \end{vmatrix}, \quad (p=1,2,\dots)$$

where the first, second and third matrices correspond to  $Q(\theta)$ ,  $R_1$  and  $R_3$  respectively. The product table is listed below.

#### Product Table, $T_4$

$$\gamma_{01}: a_1, b_1;$$

$$a_1b_1, a_2b_2, a_3b_3, a_4b_4,$$

$$a_{m1}b_{m2}+a_{m2}b_{m1}, A_{m1}B_{m2}+A_{m2}B_{m1}, \quad (m=1,2,\dots);$$

$$\gamma_{02}: a_2, b_2;$$

$$a_1b_2, a_2b_1, a_3b_4, a_4b_3,$$

$$a_{m1}B_{m2}+a_{m2}B_{m1}, A_{m1}b_{m2}+A_{m2}b_{m1}, \quad (m=1,2,\dots);$$

$$\gamma_{03}: a_3, b_3;$$

$$a_1b_3, a_2b_4, a_3b_1, a_4b_2,$$

$$a_{m1}b_{m2}-a_{m2}b_{m1}, A_{m1}B_{m2}-A_{m2}B_{m1}, \quad (m=1,2,\dots);$$

$$\gamma_{04}: a_4, b_4;$$

$$a_1b_4, a_2b_3, a_3b_2, a_4b_1,$$

$$a_{m1}B_{m2}-a_{m2}B_{m1}, A_{m1}b_{m2}-A_{m2}b_{m1}, \quad (m=1,2,\dots);$$

(cont'd)

Product Table,  $T_4$  (cont'd)

$$\begin{aligned}
 \gamma_p: & \quad \|a_{p1}, a_{p2}\|^T, \|b_{p1}, b_{p2}\|^T ; \\
 & \quad \|a_1 b_{p1}, a_1 b_{p2}\|^T, \|a_{p1} b_1, a_{p2} b_1\|^T , \\
 & \quad \|a_2 b_{p1}, a_2 b_{p2}\|^T, \|A_{p1} b_2, A_{p2} b_2\|^T , \\
 & \quad \|a_3 b_{p1}, -a_3 b_{p2}\|^T, \|a_{p1} b_3, -a_{p2} b_3\|^T , \\
 & \quad \|a_4 b_{p1}, -a_4 b_{p2}\|^T, \|A_{p1} b_4, -A_{p2} b_4\|^T , \\
 & \quad \|a_{m1} b_{n1}, a_{m2} b_{n2}\|^T, \|A_{m1} b_{n1}, A_{m2} b_{n2}\|^T , \quad (m, n=1, 2, \dots; m+n=p) , \\
 & \quad \|a_{m1} b_{n2}, a_{m2} b_{n1}\|^T, \|a_{n2} b_{m1}, a_{n1} b_{m2}\|^T , \quad (m, n=1, 2, \dots; m-n=p) , \\
 & \quad \|A_{m1} b_{n2}, A_{m2} b_{n1}\|^T, \|A_{n2} b_{m1}, A_{n1} b_{m2}\|^T , \quad (m, n=1, 2, \dots; m-n=p) ; \\
 \Gamma_p: & \quad \|A_{p1}, A_{p2}\|^T, \|B_{p1}, B_{p2}\|^T ; \\
 & \quad \|a_1 B_{p1}, a_1 B_{p2}\|^T, \|A_{p1} b_1, A_{p2} b_1\|^T , \\
 & \quad \|a_2 b_{p1}, a_2 b_{p2}\|^T, \|a_{p1} b_2, a_{p2} b_2\|^T , \\
 & \quad \|a_3 B_{p1}, -a_3 B_{p2}\|^T, \|A_{p1} b_3, -A_{p2} b_3\|^T , \\
 & \quad \|a_4 b_{p1}, -a_4 b_{p2}\|^T, \|a_{p1} b_4, -a_{p2} b_4\|^T , \\
 & \quad \|a_{m1} B_{n1}, a_{m2} B_{n2}\|^T, \|A_{m1} b_{n1}, A_{m2} b_{n2}\|^T , \quad (m, n=1, 2, \dots; m+n=p) , \\
 & \quad \|a_{m1} B_{n2}, a_{m2} B_{n1}\|^T, \|a_{n2} B_{m1}, a_{n1} B_{m2}\|^T , \quad (m, n=1, 2, \dots; m-n=p) , \\
 & \quad \|A_{m1} b_{n2}, A_{m2} b_{n1}\|^T, \|A_{n2} b_{m1}, A_{n1} b_{m2}\|^T , \quad (m, n=1, 2, \dots; m-n=p) .
 \end{aligned}$$

(2.2.15)

Basic Quantities,  $T_4$

$$\gamma_{01}: S_{11} + S_{22}, S_{33}$$

$$\gamma_{02}: p_3$$

$$\gamma_{03}: a_3$$

(2.2.16)

$$\gamma_{04}:$$

$$\gamma_1: \|p_1 + ip_2, -ip_1 + ip_2\|^T$$

$$\gamma_1: \|a_1 + ia_2, a_1 - ia_2\|^T, \|S_{13} + iS_{23}, -S_{13} + iS_{23}\|^T$$

$$\gamma_2: \|S_{11} - S_{22} + 2iS_{12}, S_{11} - S_{22} - 2iS_{12}\|^T$$

(v) The group  $T_5$ .

The group  $T_5$  is comprised of the matrices  $\underline{Q}(\theta)$  and  $\underline{D}_2 \underline{Q}(\theta)$  where  $0 \leq \theta < 2\pi$  and where

$$\underline{Q}(\theta) = \begin{pmatrix} \cos\theta & \sin\theta & 0 \\ -\sin\theta & \cos\theta & 0 \\ 0 & 0 & 1 \end{pmatrix}, \quad \underline{D}_2 = \text{diag}(-1, 1, -1). \quad (2.2.17)$$

The irreducible representations associated with the group  $T_5$  are defined by listing the matrices corresponding to the group elements  $\underline{Q}(\theta)$  and  $\underline{D}_2$ . We denote the irreducible representations by

$$\gamma_0: 1, 1$$

$$\gamma_0: 1, -1$$

(2.2.18)

$$\gamma_p: \begin{pmatrix} e^{-ip\theta} & \\ & 0, e^{ip\theta} \end{pmatrix}, \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}, \quad (p=1, 2, \dots)$$

where the first and second matrices correspond to  $Q(\theta)$  and  $D_2$  respectively. We note that the irreducible representations (2.2.18) are the same as those appearing in (2.2.6). The product table will then be the same as the product table for  $T_2$  which is again listed below.

Product Table,  $T_5$

$$\begin{aligned}
 \gamma_p: & a_0, b_0; \\
 & a_0 b_0, A_0 B_0 \\
 & a_{m1} b_{m2} + a_{m2} b_{m1}, \quad (m=1, 2, \dots); \\
 \Gamma_0: & A_0, B_0; \\
 & a_0 B_0, A_0 b_0, \\
 & a_{m1} b_{m2} - a_{m2} b_{m1}, \quad (m=1, 2, \dots) \quad (2.2.19) \\
 \gamma_p: & \|a_{p1}, a_{p2}\|^T, \|b_{p1}, b_{p2}\|^T; \\
 & \|A_0 b_{p1}, -A_0 b_{p2}\|^T, \|a_{p1} B_0, -a_{p2} B_0\|^T, \\
 & \|a_0 b_{p1}, a_0 b_{p2}\|^T, \|a_{p1} b_0, a_{p2} b_0\|^T, \\
 & \|a_{m1} b_{n1}, a_{m2} b_{n2}\|^T, \quad (m, n=1, 2, \dots; m+n=p) \\
 & \|a_{m1} b_{n2}, a_{m2} b_{n1}\|^T, \|a_{n2} b_{m1}, a_{n1} b_{m2}\|^T, \quad (m, n=1, 2, \dots; m-n=p).
 \end{aligned}$$

Basic Quantities,  $T_5$

$$\begin{aligned}
 \gamma_0: & S_{11} + S_{22}, S_{33} \\
 \Gamma_0: & p_3, a_3 \\
 \gamma_1: & \|p_1 + ip_2, -p_1 + ip_2\|^T, \|a_1 + ia_2, -a_1 + ia_2\|^T, \|S_{13} + iS_{23}, S_{13} - iS_{23}\|^T \\
 \gamma_2: & \|S_{11} - S_{22} + 2is_{12}, S_{11} - S_{22} - 2is_{12}\|^T \quad (2.2.20)
 \end{aligned}$$

## 2.3 Application

In this section, we give some examples of the application of the results derived above to the generation of non-linear constitutive expressions. We first consider the problem of determining the form of a second-order tensor-valued function

$$T_{ij} = C_{ijklm} X_k X_l X_m \quad (2.3.1)$$

which is of degree three in the components of a polar vector  $x_i$  and which is invariant under the group  $T_1$ . From the table entitled Basic Quantities  $T_1$ , we see that

$$t_{11}+t_{22}, t_{33}, t_{13}+it_{23}, t_{13}-it_{23}, t_{11}-t_{22}+2it_{12}, t_{11}-t_{22}-2it_{12} \quad (2.3.2)$$

belong to  $\gamma_0, \gamma_0, \gamma_1, \Gamma_1, \gamma_2, \Gamma_2$  respectively and that

$$x_3, x_1+ix_2, x_1-ix_2 \quad (2.3.3)$$

belong to  $\gamma_0, \gamma_1, \Gamma_1$  respectively. Upon employing the Product Table  $T_1$  twice, we see that

$$\begin{aligned} & x_3^3, x_3(x_1^2+x_2^2), x_3^2(x_1+ix_2), (x_1^2+x_2^2)(x_1+ix_2), x_3^2(x_1-ix_2) \\ & (x_1^2+x_2^2)(x_1-ix_2), x_3(x_1^2-x_2^2+2ix_1x_2), x_3(x_1^2-x_2^2-2ix_1x_2), \\ & (x_1+ix_2)^3, (x_1-ix_2)^3 \end{aligned} \quad (2.3.4)$$

belong to  $\gamma_0, \gamma_0, \gamma_1, \gamma_1, \Gamma_1, \Gamma_1, \gamma_2, \Gamma_2, \gamma_3, \Gamma_3$  respectively. Each of the



quantities in (2.3.2) which belongs to a representation  $\gamma_p$  (say) is expressible as a linear combination of the quantities in (2.3.4) which belong to  $\gamma_p$ . Thus, we have

$$\begin{aligned} \begin{vmatrix} t_{11}+t_{22} \\ t_{33} \end{vmatrix} &= \begin{vmatrix} c_1, c_2 \\ c_3, c_4 \end{vmatrix} \begin{vmatrix} x_3^3 \\ x_3(x_1^2+x_2^2) \end{vmatrix}, \\ t_{13}+it_{23} &= c_5 x_3^2(x_1+ix_2) + c_6(x_1^2+x_2^2)(x_1+ix_2), \\ t_{13}-it_{23} &= \bar{c}_5 x_3^2(x_1-ix_2) + \bar{c}_6(x_1^2+x_2^2)(x_1-ix_2), \\ t_{11}-t_{22}+2it_{12} &= c_7 x_3(x_1^2-x_2^2+2ix_1x_2), \\ t_{11}-t_{22}-2it_{12} &= \bar{c}_7 x_3(x_1^2-x_2^2-2ix_1x_2) \end{aligned} \quad (2.3.5)$$

where  $\bar{c}_5, \dots, \bar{c}_7$  denote the complex conjugates of  $c_5, \dots, c_7$ .

We next consider the problem of determining the form of the polar vector-valued function

$$x_i = c_{ijk} S_{jk} + c_{ijklm} S_{jk} S_{lm} \quad (2.3.6)$$

of the symmetric second-order tensor  $S_{ij}$  which is invariant under the group  $T_2$ . We employ the notation

$$\begin{aligned} S_1 &= S_{11}+S_{22}, \quad S_2 = S_{33}, \quad S_3 = S_{13}+iS_{23}, \quad S_4 = -S_{13}+iS_{23}, \\ S_5 &= S_{11}-S_{22}+2iS_{12}, \quad S_6 = S_{11}-S_{22}-2iS_{12}. \end{aligned} \quad (2.3.7)$$

We note that  $S_4 = -\bar{S}_3$  and  $S_6 = \bar{S}_5$ . From the table entitled

Basic Quantities  $T_2$  , we see that

$$x_3, \|x_1+ix_2, -x_1+ix_2\|^T \quad (2.3.8)$$

belong to  $\gamma_0$  and  $\gamma_1$  respectively and that

$$s_1, s_2, \|s_3, s_4\|^T, \|s_5, s_6\|^T \quad (2.3.9)$$

belong to  $\gamma_0, \gamma_0, \gamma_1$  and  $\gamma_2$  respectively. In (2.3.9), we have used the notation (2.3.7). Upon employing Product Table  $T_2$  , we see that the 21 products of degree two in the  $s_i (i=1, \dots, 6)$  belong to the representations listed below.

$$\begin{aligned} \gamma_0: & s_1^2, s_2^2, s_1 s_2, s_3 s_4, s_5 s_6 \\ \gamma_1: & s_1 \|s_3, s_4\|^T, s_2 \|s_3, s_4\|^T, \|s_4 s_5, s_3 s_6\|^T \\ \gamma_2: & s_1 \|s_5, s_6\|^T, s_2 \|s_5, s_6\|^T, \|s_3^2, s_4^2\|^T \\ \gamma_3: & \|s_3 s_5, s_4 s_6\|^T \\ \gamma_4: & \|s_5^2, s_6^2\|^T \end{aligned} \quad (2.3.10)$$

The constitutive equation (2.3.6) may then be written as

$$x_3 = c_1 s_1 + c_2 s_2 + c_3 s_1^2 + c_4 s_2^2 + c_5 s_1 s_2 + c_6 s_3 s_4 + c_7 s_5 s_6,$$

$$\begin{aligned} \begin{vmatrix} x_1+ix_2 \\ -x_1+ix_2 \end{vmatrix} &= \begin{vmatrix} c_8, 0 \\ 0, c_8 \end{vmatrix} \begin{vmatrix} s_3 \\ s_4 \end{vmatrix} + \begin{vmatrix} c_9, 0 \\ 0, c_9 \end{vmatrix} \begin{vmatrix} s_1 s_3 \\ s_1 s_4 \end{vmatrix} \\ &+ \begin{vmatrix} c_{10}, 0 \\ 0, c_{10} \end{vmatrix} \begin{vmatrix} s_2 s_3 \\ s_2 s_4 \end{vmatrix} + \begin{vmatrix} c_{11}, 0 \\ 0, c_{11} \end{vmatrix} \begin{vmatrix} s_4 s_5 \\ s_3 s_6 \end{vmatrix}. \end{aligned} \quad (2.3.11)$$

Since  $-x_1 + ix_2 = -(\overline{x_1 + ix_2})$  and  $S_4 = -\bar{S}_3$ , we see that  $c_8 = \bar{c}_8$  which implies that  $c_8$  is a real number. Similarly, we see that  $c_9$ ,  $c_{10}$  and  $c_{11}$  are also real numbers.

We next consider the problem of determining the form of the polar vector-valued function

$$x_1 = c_{ijk} S_{jk} + c_{ijk\ell m} S_{jk} S_{\ell m} \quad (2.3.12)$$

and the axial vector-valued function

$$a_i = d_{ijk} S_{jk} + d_{ijk\ell m} S_{jk} S_{\ell m} \quad (2.3.13)$$

of the symmetric second-order tensor  $S_{ij}$  which is invariant under the group  $T_3$ . We employ the notation

$$\begin{aligned} S_1 &= S_{11} + S_{22}, \quad S_2 = S_{33}, \quad S_3 = S_{13} + iS_{23}, \quad S_4 = S_{13} - iS_{23}, \\ S_5 &= S_{11} - S_{22} + 2iS_{12}, \quad S_6 = S_{11} - S_{22} - 2iS_{12}. \end{aligned} \quad (2.3.14)$$

We note that  $S_4 = \bar{S}_3$  and  $S_6 = \bar{S}_5$ . From the table entitled Basic Quantities  $T_3$ , we see that

$$x_3, x_1 + ix_2, x_1 - ix_2 \quad (2.3.15)$$

belong to  $\Gamma_0, \gamma_1, \bar{\gamma}_1$  respectively, that

$$a_3, a_1 + ia_2, a_1 - ia_2 \quad (2.3.16)$$

belong to  $\gamma_0, \Gamma_1, \bar{\Gamma}_1$  respectively and that

$$S_1, S_2, S_3, S_4, S_5, S_6 \quad (2.3.17)$$

belong to  $\gamma_0, \gamma_0, \Gamma_1, \bar{\Gamma}_1, \gamma_2, \bar{\gamma}_2$  respectively. Upon employing Product Table  $T_3$ , we see that the 21 products of degree 2 in the  $S_i (i=1, \dots, 6)$  belong to the representations listed below.

$$\begin{aligned} \gamma_0: & S_1^2, S_2^2, S_1S_2, S_3S_4, S_5S_6 \\ \Gamma_1: & S_1S_3, S_2S_3, S_4S_5 \\ \bar{\Gamma}_1: & S_1S_4, S_2S_4, S_3S_6 \\ \gamma_2: & S_1S_5, S_2S_5, S_3^2 \\ \bar{\gamma}_2: & S_1S_6, S_2S_6, S_4^2 \\ \Gamma_3: & S_3S_5 \\ \Gamma_3: & S_4S_6 \\ \gamma_4: & S_5^2 \\ \bar{\gamma}_4: & S_6^2 \end{aligned} \quad (2.3.18)$$

With (2.3.15), ..., (2.3.18), we see that there are no terms of degrees 1 or 2 in the  $S_i (i=1, \dots, 6)$  which belong to any of the representations to which  $x_3, x_1+ix_2, x_1-ix_2$  belong. This implies that a constitutive expression of the form (2.3.12) is ruled out by symmetry considerations. The constitutive expression (2.3.13) may be written as

$$a_3 = d_1 S_1 + d_2 S_2 + d_3 S_1^2 + d_4 S_2^2 + d_5 S_1 S_2 + d_6 S_3 S_4 + d_7 S_5 S_6 ,$$

$$a_1 + ia_2 = d_8 S_3 + d_9 S_1 S_3 + d_{10} S_2 S_3 + d_{11} S_4 S_5 , \quad (2.3.19)$$

$$a_1 - ia_2 = \bar{d}_8 S_4 + \bar{d}_9 S_1 S_4 + \bar{d}_{10} S_2 S_4 + \bar{d}_{11} S_3 S_6 .$$

With the notation  $d_8 = e_8 + if_8, \dots, d_{11} = e_{11} + if_{11}$  , we see from (2.3.14) that (2.3.19)<sub>2,3</sub> may be written as

$$\begin{pmatrix} a_1 \\ a_2 \end{pmatrix} = \begin{pmatrix} e_8, -f_8 \\ f_8, e_8 \end{pmatrix} \begin{pmatrix} S_{13} \\ S_{23} \end{pmatrix} + \dots + \begin{pmatrix} e_{11}, -f_{11} \\ f_{11}, e_{11} \end{pmatrix} \begin{pmatrix} (S_{11} - S_{22})S_{13} + 2S_{12}S_{23} \\ -(S_{11} - S_{22})S_{13} + 2S_{12}S_{23} \end{pmatrix} . \quad (2.3.20)$$

### 3. The General Expression for Vector-Valued and Second-Order Symmetric Tensor-Valued Form-Invariant Functions

Let  $G_{ij}$  denote a symmetric second-order tensor. The functions  $W(G_{ij}), P_{\ell}(G_{ij}), T_{k\ell}(G_{ij})$  are said to be scalar-valued, vector-valued and second-order symmetric tensor-valued functions which are invariant under a group  $\Gamma$  if

$$\begin{aligned} W(\underline{Q}\underline{G}\underline{Q}^T) &= W(\underline{G}) \\ P_{\ell}(\underline{Q}\underline{G}\underline{Q}^T) &= Q_{\ell m} P_m(\underline{G}) \\ T_{k\ell}(\underline{Q}\underline{G}\underline{Q}^T) &= Q_{km} Q_{\ell n} T_{mn}(\underline{G}) \end{aligned} \quad (3.0.1)$$

for all  $\underline{Q}$  such that  $\underline{Q}$  belongs to the group  $\Gamma$ . The determination of the general form of such functions is essential for constructing constitutive equations which express explicitly the symmetry of the material. If we consider  $W, P_{\ell}, T_{k\ell}$  to be polynomial functions in the  $G_{ij}$ , then we may determine canonical expressions for  $W(\underline{G}), P_{\ell}(\underline{G})$  and  $T_{k\ell}(\underline{G})$  of the forms

$$\begin{aligned} W &= \sum C_{i_1 i_2 \dots i_n} I_1^{i_1} I_2^{i_2} \dots I_n^{i_n} \\ \underline{P} &= \alpha_1 \underline{J}_1 + \dots + \alpha_m \underline{J}_m, \quad \underline{P} = P_{\ell} (\ell=1,2,3) \\ \underline{T} &= \beta_1 \underline{N}_1 + \dots + \beta_r \underline{N}_r, \quad \underline{T} = T_{k\ell} (k,\ell=1,2,3) \end{aligned} \quad (3.0.2)$$

where the  $\alpha_1, \dots, \beta_r$  are polynomials in the elements  $I_1, \dots, I_n$  of an integrity basis for functions of  $\underline{G}$  invariant under  $\Gamma$  and where  $\underline{J}_1, \dots, \underline{J}_m, \underline{N}_1, \dots, \underline{N}_r$  are vector and second-order tensor-valued functions which are invariant under  $\Gamma$ .

It frequently happens that polynomial relations exist between the set of invariants which form an integrity basis. Such relations are called syzygies. Smith [ 8 ] has shown that, for each crystal class, one can make use of the syzygies between the  $I_1, \dots, I_n$  to express  $W$  in the form

$$W = S_0 + S_i L_i + S_{ij} L_i L_j \quad (i, j = 1, 2, \dots, n-6)$$

where the  $S_0, \dots, S_{ij}$  are polynomials in six functionally independent invariants  $K_1, K_2, \dots, K_6$  chosen from the integrity basis  $I_1, \dots, I_n$  associated with the crystal class considered and where  $L_1, \dots, L_{n-6}$  are the remaining  $n-6$  elements of this basis. It will be shown in this section that similar results may be obtained for vector-valued and second-order symmetric tensor-valued form-invariant functions.

The symmetry properties of the 32 crystallographic groups are defined in terms of the matrices  $I, C, R_1, R_2, R_3, \dots, M_1, M_2$  which are listed below

$$\begin{aligned}
I &= \text{diag}(1,1,1) \quad , \quad C = \text{diag}(-1,-1,-1) \quad , \\
R_1 &= \text{diag}(-1,1,1) \quad , \quad R_2 = \text{diag}(1,-1,1) \quad , \quad R_3 = \text{diag}(1,1,-1) \quad , \\
D_1 &= \text{diag}(1,-1,-1) \quad , \quad D_2 = \text{diag}(-1,1,-1) \quad , \quad D_3 = \text{diag}(-1,-1,1) \quad , \\
&\hspace{25em} (3.0.4)
\end{aligned}$$

$$T_1 = \begin{vmatrix} 1 & 0 & 0 \\ 0 & 0 & 1 \\ 0 & 1 & 0 \end{vmatrix} \quad , \quad T_2 = \begin{vmatrix} 0 & 0 & 1 \\ 0 & 1 & 0 \\ 1 & 0 & 0 \end{vmatrix} \quad , \quad T_3 = \begin{vmatrix} 0 & 1 & 0 \\ 1 & 0 & 0 \\ 0 & 0 & 1 \end{vmatrix}$$

$$S_1 = \begin{vmatrix} -1/2 & \sqrt{3}/2 & 0 \\ -\sqrt{3}/2 & -1/2 & 0 \\ 0 & 0 & 1 \end{vmatrix} \quad , \quad S_2 = \begin{vmatrix} -1/2 & -\sqrt{3}/2 & 0 \\ \sqrt{3}/2 & -1/2 & 0 \\ 0 & 0 & 1 \end{vmatrix} \quad ,$$

$$M_1 = \begin{vmatrix} 0 & 1 & 0 \\ 0 & 0 & 1 \\ 1 & 0 & 0 \end{vmatrix} \quad , \quad M_2 = \begin{vmatrix} 0 & 0 & 1 \\ 1 & 0 & 0 \\ 0 & 1 & 0 \end{vmatrix} \quad .$$

Since the techniques employed here involve the use of generating function, we outline in §3.1 some theoretical background concerning generating functions. The step-by-step illustration of the procedure we employ is shown in §3.2. In §3.3, we list the results thus obtained for each of 32 crystal classes.

### 3.1. Generating functions

Let  $\tilde{x}$  be a column vector consisting of all the independent components of the quantities (vectors, second-order tensors, ...) being considered. For example, for the symmetric second-order tensor  $G_{ij}$  ,

$$\tilde{x} = (G_{11}, G_{22}, G_{33}, G_{23}, G_{31}, G_{12})^T .$$



Given a group  $\Gamma$ , for any  $S \in \Gamma$ , the result of applying  $S$  to  $\underline{x}$  will be another vector  $\underline{x}'$  in general, and we may write  $\underline{x}'$  as

$$\underline{x}' = \underline{A}(s)\underline{x}, \quad S \in \Gamma \quad (3.1.1)$$

where  $\underline{A}(s)$  is an  $n \times n$  matrix. All such  $\underline{A}(s)$  form an  $n$ -dimensional matrix representation of the group  $\Gamma$ . According to group representation theory, for a finite group  $\Gamma$ , every representation is equivalent to a unitary representation. Thus we may assume that our representation  $\{\underline{A}\}$  is a unitary representation.

When  $\underline{x}$  undergoes the linear transformation

$$x'_i = \sum_k \underline{A}_{ik} x_k, \quad \underline{A} = \|\underline{A}_{ik}\| \quad (3.1.2)$$

the monomials of degree  $f$

$$x_1^{r_1} x_2^{r_2} \dots x_n^{r_n}, \quad (r_1 + r_2 + \dots + r_n = f) \quad (3.1.3)$$

undergo the corresponding linear transformation  $\underline{A}_f$ , where  $\underline{A}_f$  is the symmetrized  $f^{\text{th}}$  Kronecker product of  $\underline{A}$ . Since  $\underline{A}$  is unitary,  $\underline{A}_f$  can always be diagonalized; i.e., we can always find a matrix  $\underline{U}$  such that

$$\underline{U}^{-1} \underline{A}_f \underline{U} = \underline{\epsilon} = \text{diag}(\epsilon_1, \epsilon_2, \dots, \epsilon_n). \quad (3.1.4)$$

Assuming  $\underline{A}$  to be in the normal form  $\underline{\epsilon}$ , it is easy to see that under the influence of  $\underline{A}$ , each monomial in (3.1.3) is multiplied by the factor

$$\epsilon_1^{r_1} \epsilon_2^{r_2} \dots \epsilon_n^{r_n} ,$$

i.e., the corresponding transformation  $A_{\sim f}$  is also in diagonal form.

Therefore

$$\text{Tr} A_{\sim f} = \sum \epsilon_1^{r_1} \epsilon_2^{r_2} \dots \epsilon_n^{r_n} \equiv P_f \quad (3.1.5)$$

where the sum is over all non-negative integers  $r_1, \dots, r_n$  whose sum is  $f$ .

It is well known that

$$\frac{1}{1 - \epsilon z} = \sum_{r=0}^{\infty} \epsilon^r z^r , \quad |z| < 1 . \quad (3.1.6)$$

Thus

$$\frac{1}{(1 - \epsilon_1 z)(1 - \epsilon_2 z) \dots (1 - \epsilon_n z)} = \sum_{f=0}^{\infty} P_f z^f \quad (3.1.7)$$

where  $P_f$  is defined by (3.1.5). Since  $\det(E - zA) = \det U^{-1}(E - zA)U = \det(E - zU^{-1}AU) = (1 - \epsilon_1 z)(1 - \epsilon_2 z) \dots (1 - \epsilon_n z)$ , we have

$$\frac{1}{\det(E - zA)} = \sum_{f=0}^{\infty} P_f z^f . \quad (3.1.8)$$

If  $\{A\}$  is a representation of the group  $\Gamma$ ,  $\{A_{\sim f}\}$  is also a representation of  $\Gamma$ . The number of times the  $\nu^{\text{th}}$  irreducible representation  $\Gamma_{\nu}$  occurs in  $\{A_{\sim f}\}$  is the same as the number of bases for  $\Gamma_{\nu}$  which are linear combinations of the monomials

$$x_1^{r_1} x_2^{r_2} \dots x_n^{r_n}, \quad r_1 + r_2 + \dots + r_n = f.$$

Since the bases thus obtained are linearly independent polynomial functions of degree  $f$  in the  $x_j$ , we have the following important result.

The number  $a_f^\nu$  of linearly independent functions of degree  $f$  in the  $x_j$  which belong to  $\Gamma_\nu$  is given by

$$\sum_{f=0}^{\infty} a_f^\nu z^f = \frac{1}{g} \sum_{S \in \Gamma} \frac{\bar{\chi}^{(\nu)}(s)}{\det[\tilde{E} - z\tilde{A}(s)]} \quad (3.1.9)$$

where  $g$  is the order of group  $\Gamma$ ,  $\bar{\chi}^{(\nu)}$  is the complex conjugate of the  $\nu^{\text{th}}$  simple character and  $\{\tilde{A}\}$  is the matrix representation of  $\Gamma$ .

In group representation theory, a function  $F_\nu(x_j)$  is said to belong to the  $\nu^{\text{th}}$  irreducible representation  $\Gamma_\nu$  if  $F_\nu$  is a base function for the  $\nu^{\text{th}}$  irreducible representation. For the sake of convenience, we call such a function  $F_\nu$  a  $\Gamma_\nu$ -type function.

Suppose that  $J_k(x_j)$  is a  $\Gamma_\nu$ -type function. Then for any scalar-valued invariant  $\alpha(x_j)$ ,  $\alpha J_k$  is also a  $\Gamma_\nu$ -type function. Given that  $J_1, \dots, J_m$  form a basis for  $\Gamma_\nu$ -type functions, each  $\Gamma_\nu$ -type function  $F_\nu$  may be expressed in the following form

$$F_\nu = \alpha_1 J_1 + \alpha_2 J_2 + \dots + \alpha_m J_m \quad (3.1.10)$$

where the  $\alpha_k$  are of the form (see eqn. (3.0.3))

$$\alpha_k = S_0 + S_i L_i + S_{ij} L_i L_j, \quad (i, j=1, \dots, n-6) \quad (3.1.11)$$

if  $\underline{x} = (G_{11}, G_{22}, G_{33}, G_{23}, G_{31}, G_{12})^T$ . Substituting (3.1.11) into (3.1.10), we have

$$F_v = S_{k\sim k} J_k + S_{ik} L_i J_k + S_{ijk} L_i L_j J_k, \quad (i, j=1, \dots, n-6; k=1, \dots, m) \quad (3.1.12)$$

where the  $S_k, \dots, S_{ijk}$  are polynomials in the quantities  $K_1, \dots, K_6$  and where  $K_1, \dots, K_6, L_1, \dots, L_{n-6}$  form an integrity basis.

In general, only a few terms in  $L_i J_k$  and  $L_i L_j J_k$  are needed, the others being redundant. The question is, how many terms of the form  $L_i J_k$  or  $L_i L_j J_k$  are needed. The generating function can give us the exact answer.

Starting from (3.1.9), the number of linearly independent  $\Gamma_v$ -type functions of degree  $f$  is given by the coefficient of  $z^f$  in the expansion

$$\frac{1}{9} \sum_{S \in \Gamma} \frac{\bar{\chi}^{(v)}(s)}{\det[\tilde{E} - z\tilde{A}(s)]} = \sum_{f=0}^{\infty} a_f^v z^f.$$

Suppose that the 6 functionally independent invariants  $K_1, \dots, K_6$  are of degree  $i_1, \dots, i_6$  in  $\underline{x}$  respectively. Then

$$\sum_{f=0}^{\infty} a_f^v z^f = \frac{Z}{(1-z^{i_1})(1-z^{i_2}) \dots (1-z^{i_6})} \quad (3.1.13)$$

where

$$Z = \left( \frac{1}{9} \sum_{S \in \Gamma} \frac{\bar{\chi}^{(v)}(s)}{\det[\tilde{E} - z\tilde{A}(s)]} \right) \cdot (1-z^{i_1})(1-z^{i_2}) \dots (1-z^{i_6}). \quad (3.1.14)$$

We can choose the invariants  $K_i (i=1,2,\dots,6)$  such that  $Z$  is a polynomial in  $Z$ , i.e.,

$$Z = \sum_{p=0}^N b_p z^p \quad (3.1.15)$$

If this is the case, then  $b_p$  gives the number of linearly independent terms  $L_i J_k$  and  $L_i L_j J_k$  appearing in the canonical expression for  $F_v$  which are of degree  $p$  in the  $x_j$ . In general, the number  $\sum b_p$  is much less than the number of terms  $L_i J_k$  and  $L_i L_j J_k$  appearing in (3.1.12). We can thus simplify the canonical expression for  $F_v$  enormously.

### 3.2. Application of the generating function technique

In this section, we will show how to use the generating function technique to obtain the general expression for vector-valued and second-order symmetric tensor-valued form-invariant functions. The group considered in the example is a crystallographic group and hence the results given in [ 6 ], [ 9 ] may be used. In the example, we will list all the syzygies employed.

Example: Tetragonal-scalenohedral class,  $D_{2d}$

For this group, the irreducible representations are given below. The matrices  $I, D_1, \dots, D_{13}$  comprising the group  $D_{2d}$  are defined in [ 6 ].

Table 3.1 Irreducible Representations:  $D_{2d}$

	$\tilde{I}$	$\tilde{D}_1$	$\tilde{D}_2$	$\tilde{D}_3$	$\tilde{T}_3$	$\tilde{D}_1\tilde{T}_3$	$\tilde{D}_2\tilde{T}_3$	$\tilde{D}_3\tilde{T}_3$
$\Gamma_1$	1	1	1	1	1	1	1	1
$\Gamma_2$	1	-1	-1	1	-1	1	1	-1
$\Gamma_3$	1	-1	-1	1	1	-1	-1	1
$\Gamma_4$	1	1	1	1	-1	-1	-1	-1
$\Gamma_5$	$\tilde{E}$	$\tilde{F}$	$-\tilde{F}$	$-\tilde{E}$	$\tilde{K}$	$\tilde{L}$	$-\tilde{L}$	$-\tilde{K}$

The matrices  $\tilde{E}, \dots, \tilde{L}$  appearing in Table 3.1 are defined by

$$\tilde{E} = \begin{vmatrix} 1 & 0 \\ 0 & 1 \end{vmatrix}, \quad \tilde{F} = \begin{vmatrix} 1 & 0 \\ 0 & -1 \end{vmatrix}, \quad \tilde{K} = \begin{vmatrix} 0 & 1 \\ 1 & 0 \end{vmatrix}, \quad \tilde{L} = \begin{vmatrix} 0 & 1 \\ -1 & 0 \end{vmatrix}.$$

The basic quantities are listed in Table 3.2. By basic quantities, we mean the quantities consisting of linear combinations of the components of  $G_{ij}, P_k, T_{kl}$  which form the bases for the representations  $\Gamma_v$ .

Table 3.2 Basic Quantities:  $D_{2d}$

$\Gamma_1$	$G_{33}, G_{11}+G_{22} ; T_{33}, T_{11}+T_{22}$
$\Gamma_2$	
$\Gamma_3$	$G_{12} ; P_3 ; T_{12}$
$\Gamma_4$	$G_{11}-G_{22} ; T_{11}-T_{22}$
$\Gamma_5$	$(G_{23}, G_{31})^T ; (P_1, P_2)^T ; (T_{23}, T_{31})^T$

The expressions for  $\det(\underline{E}-x\underline{A})$  for the matrices  $\underline{A}$  comprising the group  $D_{2d}$  are given in Table 3.3. The integrity basis for this group [ 8 ] is given by

$$K_1 = G_{11} + G_{22} , K_2 = G_{11}G_{22} , K_3 = G_{33} , K_4 = G_{23}^2 + G_{31}^2 ,$$

$$K_5 = G_{23}^2 G_{31}^2 , K_6 = G_{12}^2 , L_1 = G_{23}G_{31}G_{12} , L_2 = (G_{11} - G_{22})(G_{31}^2 - G_{23}^2) .$$

Table 3.3  $\det(\underline{E}-x\underline{A})$ :  $D_{2d}$

$\underline{A}$	$\det(\underline{E}-x\underline{A})$
I	$(1-x)^6$
$D_1, D_2$	$(1-x)^2(1-x^2)^2$
$D_3$	$(1-x)^2(1-x^2)^2$
$T_3, D_3T_3$	$(1-x)^2(1-x^2)^2$
$D_1T_3, D_2T_3$	$(1-x^2)(1-x^4)$

The generating function is in the form

$$GF = \frac{Z}{(1-x)^2(1-x^2)^3(1-x^4)} \quad (3.2.1)$$

where  $Z$  is given in Table 3.4.

Table 3.4      Z:  $D_{2d}$

	Z
$\Gamma_1$	$1+2x^3+x^6$
$\Gamma_2$	$x^2+2x^3+x^4$
$\Gamma_3$	$x+x^2+x^4+x^5$
$\Gamma_4$	$x+x^2+x^4+x^5$
$\Gamma_5$	$x+2x^2+2x^3+2x^4+x^5$

(1) General expression for  $\Gamma_1$  -type functions.

From Table 3.4, we have

$$Z = 1 + 2x^3 + x^6$$

The corresponding terms are

$$\begin{aligned} x^3: & \quad L_1 = G_{23}G_{31}G_{12} , \\ x^3: & \quad L_2 = (G_{11}-G_{22})(G_{31}^2-G_{23}^2) , \\ x^6: & \quad L_1L_2 . \end{aligned}$$

We then have the general expression for  $\Gamma_1$  -type functions (invariants)

$$F_1 = S_0 + S_1L_1 + S_2L_2 + S_3L_1L_2 \quad (3.2.2)$$

where the  $S_0, \dots, S_3$  are polynomials in the quantities  $K_1, \dots, K_6$  .

(2) General expression for  $\Gamma_3$  -type functions.

From Table 3.4, we have

$$Z = x + x^2 + x^4 + x^5 .$$



The corresponding terms are

$$\begin{aligned} x : I_1 &= G_{12} , \\ x^2 : I_2 &= G_{23}G_{31} , \\ x^4 : L_2 I_1 , \\ x^5 : L_2 I_2 . \end{aligned}$$

We have the following identities:

$$\begin{aligned} L_1 I_1 &= K_6 I_2 , \quad L_1 L_2 I_1 = K_6 L_2 I_2 , \\ L_1 I_2 &= K_5 I_1 , \quad L_1 L_2 I_2 = K_5 L_2 I_1 . \end{aligned}$$

The general expression for  $\Gamma_3$  -type functions is then given by

$$F_3 = S_1 I_1 + S_2 I_2 + S_3 L_2 I_1 + S_4 L_2 I_2 \quad (3.2.3)$$

where the  $S_1, \dots, S_4$  are polynomials in the quantities  $K_1, \dots, K_6$  .

(3) General expression for  $\Gamma_4$  -type functions.

From Table 3.4, we have

$$Z = x + x^2 + x^4 + x^5 .$$

The corresponding terms are

$$\begin{aligned} x : J_1 &= G_{11} - G_{22} , \\ x^2 : J_2 &= G_{31}^2 - G_{23}^2 , \\ x^4 : L_1 J_1 , \\ x^5 : L_1 J_2 . \end{aligned}$$

We have the following identities:

$$L_2 J_1 = (K_1^2 - 4K_2) J_2, \quad L_1 L_2 J_1 = (K_1^2 - 4K_2) L_1 J_2,$$

$$L_2 J_2 = (K_4^2 - 4K_5) J_1, \quad L_1 L_2 J_2 = (K_4^2 - 4K_5) L_1 J_1.$$

Consequently, the general expression for  $\Gamma_4$ -type functions is

$$F_4 = S_1 J_1 + S_2 J_2 + S_3 L_1 J_1 + S_4 L_1 J_2 \quad (3.2.4)$$

where the  $S_1, \dots, S_4$  are polynomials in the quantities  $K_1, \dots, K_6$ .

(4) General expression for  $\Gamma_5$ -type functions.

From Table 3.4, we have

$$Z = x + 2x^2 + 2x^3 + 2x^3 + 2x^4 + x^5$$

The corresponding terms are

$$\begin{aligned} x: \quad \tilde{N}_1 &= \begin{vmatrix} G_{23} \\ G_{31} \end{vmatrix}, \\ x^2: \quad \tilde{N}_2 &= (G_{11} - G_{22}) \begin{vmatrix} -G_{23} \\ G_{31} \end{vmatrix}, \\ x^2: \quad \tilde{N}_3 &= G_{12} \begin{vmatrix} G_{31} \\ G_{23} \end{vmatrix}, \\ x^3: \quad \tilde{N}_4 &= G_{12} (G_{11} - G_{22}) \begin{vmatrix} G_{31} \\ -G_{23} \end{vmatrix}, \\ x^3: \quad \tilde{N}_5 &= G_{23} G_{31} \begin{vmatrix} G_{31} \\ G_{23} \end{vmatrix}, \\ 2x^4: \quad &L_1 \tilde{N}_1, \quad L_2 \tilde{N}_1, \\ x^5: \quad &L_1 \tilde{N}_2. \end{aligned} \quad (3.2.5)$$

We have the following identities:

$$L_{1\sim 3} = K_{5\sim 5} , \quad 2L_{1\sim 4} = K_6(L_{2\sim 1} - K_{4\sim 2}) , \quad L_{1\sim 5} = K_{5\sim 3} ,$$

$$L_{2\sim 2} = (K_1^2 - 4K_2)(K_{4\sim 1} - 2N_{\sim 5}) , \quad L_{2\sim 3} = K_{4\sim 4} + 2L_{1\sim 2} ,$$

$$L_{2\sim 4} = (K_1^2 - 4K_2)(K_{4\sim 3} - 2L_{1\sim 1}) , \quad 2L_{2\sim 5} = K_4(L_{2\sim 1} - K_{4\sim 2}) + 4K_{5\sim 2} ,$$

$$L_1 L_{2\sim 1} = K_4 L_{1\sim 2} + 2K_{5\sim 4} , \quad L_1 L_{2\sim 2} = (K_1^2 - 4K_2)(K_4 L_{1\sim 1} - 2K_{5\sim 3}) ,$$

$$2L_1 L_{2\sim 3} = K_4 K_6 (L_{2\sim 1} - K_{4\sim 2}) + 4K_5 K_{6\sim 2} ,$$

$$L_1 L_{2\sim 4} = (K_1^2 - 4K_2) K_6 (K_{4\sim 5} - 2K_{5\sim 1}) , \quad L_1 L_{2\sim 5} = K_5 (K_{5\sim 4} + 2L_{1\sim 2}) .$$

Consequently, the general expression for  $\Gamma_5$ -type functions is given by

$$F_{\sim 5} = \sum_{i=1}^5 S_i N_i + S_6 L_{1\sim 1} + S_7 L_{1\sim 2} + S_8 L_{2\sim 1} \quad (3.2.6)$$

where the  $S_1, \dots, S_8$  are polynomials in the quantities  $K_1, \dots, K_6$ .

We are now in a position to determine the general expressions for  $P_\ell$  and  $T_{k\ell}$ . For a vector-valued function  $P_\ell(G_{ij})$ , from Table 3.2, we know that  $(P_1, P_2)^T$  belongs to  $\Gamma_5$  and  $P_3$  belongs to  $\Gamma_3$ .

We then have the general expression for  $P_\ell(G_{ij})$ .

$$\begin{pmatrix} P_1 \\ P_2 \end{pmatrix} = \sum_{i=1}^5 a_i N_i + a_6 L_{1\sim 1} + a_7 L_{1\sim 2} + a_8 L_{2\sim 1} ,$$

$$P_3 = b_1 I_1 + b_2 I_2 + b_3 L_2 I_1 + b_4 L_2 I_2$$

where the quantities  $a_1, \dots, a_8$ ,  $b_1, \dots, b_4$  are polynomials in the quantities  $K_1, \dots, K_6$  and where the  $\underline{N}_1, \dots, \underline{N}_5$  are defined by (3.2.5).

For a second-order symmetric tensor-valued function  $T_{kl}(G_{ij})$ , from Table 2.2, we know that  $T_{11}+T_{22}$  and  $T_{33}$  belong to  $\Gamma_1$ ;  $T_{12}$  belongs to  $\Gamma_3$ ;  $T_{11}-T_{22}$  belongs to  $\Gamma_4$  and  $(T_{23}, T_{31})^T$  belongs to  $\Gamma_5$ . We then have the general expression for  $T_{kl}(G_{ij})$ .

$$T_{11}+T_{22} = c_0 + c_1 L_1 + c_2 L_2 + c_3 L_1 L_2 ,$$

$$T_{33} = d_0 + d_1 L_1 + d_2 L_2 + d_3 L_1 L_2$$

$$T_{12} = e_1 I_1 + e_2 I_2 + e_3 L_2 I_1 + e_4 L_2 I_2 ,$$

$$T_{11}-T_{22} = f_1 J_1 + f_2 J_2 + f_3 L_1 J_1 + f_4 L_1 J_2 ,$$

$$\begin{Bmatrix} T_{23} \\ T_{31} \end{Bmatrix} = \sum_{i=1}^5 g_i \underline{N}_i + g_6 L_1 \underline{N}_1 + g_7 L_1 \underline{N}_2 + g_8 L_2 \underline{N}_1$$

where the quantities  $c_0, \dots, c_3$ ,  $d_0, \dots, d_3$ ,  $e_1, \dots, e_4$ ,  $f_1, \dots, f_4$  and  $g_1, \dots, g_8$  are polynomials in the quantities  $K_1, \dots, K_6$ .

### 3.3 Canonical Expressions for Quantities of Type $\Gamma_v$ - the Crystal Classes

In this section, we present tables which give canonical expressions for quantities of type  $\Gamma_v$  for each of the crystal classes (except for classes  $T, T_h$  where technical difficulties arise). We see then from the examples given in 3.2 that the information in the tables given below enables us to determine the general expressions for vector-valued functions  $P_i(G_{k\ell})$  and second-order tensor-valued functions  $T_{ij}(G_{k\ell})$  which are invariant under a given crystallographic group. We list tables defining the irreducible representations  $\Gamma_v$  associated with the crystallographic groups. The characters  $\chi^{(\nu)}(A_i)$  of the irreducible representations  $\Gamma_v$  may be obtained immediately from the tables giving the irreducible representations. We also list tables giving basic quantities in terms of linear combinations of the components  $P_i, T_{ij}$  and  $G_{ij}$ . The generating functions are given by  $GF(\Gamma_v) = Z_v(x)/D(x)$ . The quantities  $Z_v$  are listed in the tables. We also tabulate the canonical expressions for quantities of type  $\Gamma_v$ . These expressions are of the forms  $a_0 + a_1 L_1 + \dots, \dots, c_1 J_1 + c_2 J_2 + \dots$  where the  $L_1, \dots, J_1$  are quantities of types  $\Gamma_1, \dots, \Gamma_v$  and where the coefficients  $a_0, a_1, \dots, c_1, c_2, \dots$  are polynomial functions of six functionally independent invariants  $K_1, \dots, K_6$ .

### 3.3.1 Pedial class, $C_1, I$ .

Since the materials belonging to this crystal class possess no symmetry properties, there are no restrictions on the form of the constitutive expressions. We have

$$P_i = P_i^*(G_{11}, G_{22}, G_{33}, G_{23}, G_{31}, G_{12}) , \quad (i=1,2,3)$$

$$T_{ij} = T_{ij}^*(G_{11}, G_{22}, G_{33}, G_{23}, G_{31}, G_{12}) , \quad (i,j=1,2,3)$$

where  $P_i^*$ ,  $T_{ij}^*$  are polynomials in the indicated arguments.

3.3.2 Pinacoidal class,  $C_i, (\underline{I}, \underline{C})$

Domatic class,  $C_s, (\underline{I}, \underline{R}_1)$

Sphenoidal class,  $C_2, (\underline{I}, \underline{D}_1)$

Table 3.5 Irreducible Representations:  $C_i, C_s, C_2$

$C_i$	$\underline{I}$	$\underline{C}$
$C_s$	$\underline{I}$	$\underline{R}_1$
$C_2$	$\underline{I}$	$\underline{D}_1$
$\Gamma_1$	1	1
$\Gamma_2$	1	-1

Table 3.6 Pinacoidal class,  $C_i$

I.R.	Basic Quantities		$Z_v$	Canonical Expressions
$\Gamma_1$	$T_{11}, T_{22}, T_{33}$ $T_{23}, T_{31}, T_{12}$	$G_{11}, G_{22}, G_{33}$ $G_{23}, G_{31}, G_{12}$	1	$a_0$
$\Gamma_2$	$P_1, P_2, P_3$		0	None

Integrity Basis:  $C_i$

$$K_1, \dots, K_6 = G_{11}, G_{22}, G_{33}, G_{23}, G_{31}, G_{12}$$

Generating Function:  $C_i$

$$GF(\Gamma_v) = \frac{Z_v}{(1-x)^6}$$

Table 3.7 Domatic class,  $C_5$

I.R.	Basic Quantities		$Z_v$	Canonical Expressions
$\Gamma_1$	$T_{11}, T_{22}, T_{33}, T_{23}$ $P_2, P_3$	$G_{11}, G_{22}, G_{33}, G_{23}$	$1+x^2$	$a_0 + a_1 L_1$
$\Gamma_2$	$T_{31}, T_{12}$ $P_1$	$G_{31}, G_{12}$	$2x$	$b_0 G_{31} + b_1 G_{12}$

Table 3.8 Sphenoidal class,  $C_2$

I.R.	Basic Quantities		$Z_v$	Canonical Expressions
$\Gamma_1$	$T_{11}, T_{22}, T_{33}, T_{23}$ $P_1$	$G_{11}, G_{22}, G_{33}, G_{23}$	$1+x^2$	$a_0 + a_1 L_1$
$\Gamma_2$	$T_{31}, T_{12}$ $P_2, P_3$	$G_{31}, G_{12}$	$2x$	$b_0 G_{31} + b_1 G_{12}$

Integrity Basis:  $C_5, C_2$

$$K_1, \dots, K_6 = G_{11}, G_{22}, G_{33}, G_{23}, G_{31}^2, G_{12}^2$$

$$L_1 = G_{23} G_{31}$$

Generating Function:  $C_5, C_2$

$$GF(\Gamma_v) = \frac{Z_v}{(1-x)^4 (1-x^2)^2}$$



3.3.3 Prismatic class,  $C_{2h}, (\underline{I}, \underline{C}, \underline{R}_1, \underline{D}_1)$

Rhombic-pyramidal class,  $C_{2v}, (\underline{I}, \underline{R}_2, \underline{R}_3, \underline{D}_1)$

Rhombic-disphenoidal class,  $D_2, (\underline{I}, \underline{D}_1, \underline{D}_2, \underline{D}_3)$

Table 3.9 Irreducible Representations:  $C_{2h}, C_{2v}, D_2$

$C_{2h}$	I	$D_1$	$R_1$	C
$C_{2v}$	I	$D_1$	$R_3$	$R_2$
$D_2$	I	$D_1$	$D_2$	$D_3$
$\Gamma_1$	1	1	1	1
$\Gamma_2$	1	1	-1	-1
$\Gamma_3$	1	-1	1	-1
$\Gamma_4$	1	-1	-1	1

Table 3.10 Prismatic class,  $C_{2h}$

I.R.	Basic Quantities		$Z_v$	Canonical Expressions
$\Gamma_1$	$T_{11}, T_{22}, T_{33}, T_{23}$	$G_{11}, G_{22}, G_{33}, G_{23}$	$1+x^2$	$a_0 + a_1 L_1$
$\Gamma_2$	$P_1$		0	None
$\Gamma_3$	$P_2, P_3$		0	None
$\Gamma_4$	$T_{31}, T_{12}$	$G_{31}, G_{12}$	$2x$	$b_0 G_{31} + b_1 G_{12}$

Integrity Basis:  $C_{2h}$

$$K_1, \dots, K_6 = G_{11}, G_{22}, G_{33}, G_{23}, G_{31}^2, G_{12}^2$$

$$L_1 = G_{31} G_{12}$$

Generating Function:  $C_{2h}$

$$GF(\Gamma_v) = \frac{Z_v}{(1-x)^4 (1-x^2)^2}$$

Table 3.11 Rhombic-pyramidal class,  $C_{2v}$ 

I.R.	Basic Quantities		$Z_v$	Canonical Expressions
$\Gamma_1$	$T_{11}, T_{22}, T_{33}; P_1$	$G_{11}, G_{22}, G_{33}$	$1+x^3$	$a_0 + a_1 L_1$
$\Gamma_2$	$T_{23}$	$G_{23}$	$x+x^2$	$b_0 G_{23} + b_1 G_{31} G_{12}$
$\Gamma_3$	$T_{12}; P_3$	$G_{12}$	$x+x^2$	$c_0 G_{12} + c_1 G_{23} G_{31}$
$\Gamma_4$	$G_{31}; P_3$	$G_{31}$	$x+x^2$	$d_0 G_{31} + d_1 G_{12} G_{23}$

Integrity Basis:  $C_{2v}$ 

$$K_1, \dots, K_6 = G_{11}, G_{22}, G_{33}, G_{23}^2, G_{31}^2, G_{12}^2$$

$$L_1 = G_{23} G_{31} G_{12}$$

Generating Function:  $C_{2v}$ 

$$GF(\Gamma_v) = \frac{Z_v}{(1-x)^3(1-x^2)^3}$$

Table 3.12 Rhombic-disphenoidal class,  $D_2$ 

I.R.	Basic Quantities		$Z_v$	Canonical Expressions
$\Gamma_1$	$T_{11}, T_{22}, T_{33}$	$G_{11}, G_{22}, G_{33}$	$1+x^3$	$a_0 + a_1 L_1$
$\Gamma_2$	$T_{23}; P_1$	$G_{23}$	$x+x^2$	$b_0 G_{23} + b_1 G_{31} G_{12}$
$\Gamma_3$	$T_{31}; P_2$	$G_{31}$	$x+x^2$	$c_0 G_{31} + c_1 G_{23} G_{12}$
$\Gamma_4$	$T_{12}; P_3$	$G_{12}$	$x+x^2$	$d_0 G_{12} + d_1 G_{23} G_{31}$

Integrity Basis:  $D_2$ 

$$K_1, \dots, K_6 = G_{11}, G_{22}, G_{33}, G_{23}^2, G_{31}^2, G_{12}^2$$

$$L_1 = G_{23} G_{31} G_{12}$$

Generating Function:  $D_2$ 

$$GF(\Gamma_v) = \frac{Z_v}{(1-x)^3(1-x^2)^3}$$

3.3.4 Rhombic-dipyramidal class,  $D_{2h}(\underline{I}, \underline{C}, \underline{R}_1, \underline{R}_2, \underline{R}_3, \underline{D}_1, \underline{D}_2, \underline{D}_3)$

Table 3.13 Irreducible Representations:  $D_{2h}$

$D_{2h}$	$\underline{I}$	$\underline{D}_1$	$\underline{D}_2$	$\underline{D}_3$	$\underline{C}$	$\underline{R}_1$	$\underline{R}_2$	$\underline{R}_3$
$\Gamma_1$	1	1	1	1	1	1	1	1
$\Gamma_2$	1	1	-1	-1	1	1	-1	-1
$\Gamma_3$	1	-1	1	-1	1	-1	1	-1
$\Gamma_4$	1	-1	-1	1	1	-1	-1	1
$\Gamma_5$	1	1	1	1	-1	-1	-1	-1
$\Gamma_6$	1	1	-1	-1	-1	-1	1	1
$\Gamma_7$	1	-1	1	-1	-1	1	-1	1
$\Gamma_8$	1	-1	-1	1	-1	1	1	-1

Table 3.14 Rhombic-dipyramidal class,  $D_{2h}$

I.R.	Basic Quantities		$Z_v$	Canonical Expressions
$\Gamma_1$	$T_{11}, T_{22}, T_{33}$	$G_{11}, G_{22}, G_{33}$	$1+x^3$	$a_0 + a_1 L_1$
$\Gamma_2$	$T_{23}$	$G_{23}$	$x+x^2$	$b_0 G_{23} + b_1 G_{31} G_{12}$
$\Gamma_3$	$T_{31}$	$G_{31}$	$x+x^2$	$c_0 G_{31} + c_1 G_{23} G_{12}$
$\Gamma_4$	$T_{12}$	$G_{12}$	$x+x^2$	$d_0 G_{12} + d_1 G_{23} G_{31}$
$\Gamma_5$			0	None
$\Gamma_6$	$P_1$		0	None
$\Gamma_7$	$P_2$		0	None
$\Gamma_8$	$P_3$		0	None

Integrity Basis:  $D_{2h}$

$$K_1, \dots, K_6 = G_{11}, G_{22}, G_{33}, G_{23}^2, G_{31}^2, G_{12}^2$$

$$L_1 = G_{23} G_{31} G_{12}$$

Generating Function:  $D_{2h}$

$$GF(\Gamma_v) = \frac{Z_v}{(1-x)^3 (1-x^2)^3}$$

3.3.5 Tetragonal-disphenoidal class,  $S_4, (\underline{I}, \underline{D}_3, \underline{D}_1\underline{T}_3, \underline{D}_2\underline{T}_3)$

Tetragonal-pyramidal class,  $C_4, (\underline{I}, \underline{D}_3, \underline{R}_1\underline{T}_3, \underline{R}_2\underline{T}_3)$

Tetragonal-dipyramidal class,  $C_{4h}, (\underline{I}, \underline{C}, \underline{R}_3, \underline{D}_3, \underline{R}_1\underline{T}_3, \underline{R}_2\underline{T}_3, \underline{D}_1\underline{T}_3, \underline{D}_2\underline{T}_3)$

Table 3.15 Irreducible Representations:  $S_4, C_4$

$S_4$	$\underline{I}$	$\underline{D}_3$	$\underline{D}_1\underline{T}_3$	$\underline{D}_2\underline{T}_3$
$C_4$	$\underline{I}$	$\underline{D}_3$	$\underline{R}_1\underline{T}_3$	$\underline{R}_2\underline{T}_3$
$\Gamma_1$	1	1	1	1
$\Gamma_2$	1	1	-1	-1
$\Gamma_3$	1	-1	i	-i
$\Gamma_4$	1	-1	-i	i

Table 3.16 Irreducible Representations:  $C_{4h}$

$C_{4h}$	$\underline{I}$	$\underline{D}_3$	$\underline{R}_1\underline{T}_3$	$\underline{R}_2\underline{T}_3$	$\underline{C}$	$\underline{R}_3$	$\underline{D}_1\underline{T}_3$	$\underline{D}_2\underline{T}_3$
$\Gamma_1$	1	1	1	1	1	1	1	1
$\Gamma_2$	1	1	-1	-1	1	1	-1	-1
$\Gamma_3$	1	-1	i	-i	1	-1	i	-i
$\Gamma_4$	1	-1	-i	i	1	-1	-i	i
$\Gamma_5$	1	1	1	1	-1	-1	-1	-1
$\Gamma_6$	1	1	-1	-1	-1	-1	1	1
$\Gamma_7$	1	-1	i	-i	-1	1	-i	i
$\Gamma_8$	1	-1	-i	i	-1	1	i	-i

Table 3.17 Tetragonal-disphenoidal class,  $S_4$

I.R.	Basic Quantities		$Z_v$
$\Gamma_1$	$T_{11}+T_{22}, T_{33}$	$G_{11}+G_{22}, G_{33}$	$1+x^2+4x^3+x^4+x^6$
$\Gamma_2$	$T_{11}-T_{22}, T_{12}$ $P_3$	$G_{11}-G_{22}, G_{12}$	$2(x+x^2+x^4+x^5)$
$\Gamma_3$	$T_{31}+iT_{23}$ $P_1-iP_2$	$G_{31}+iG_{23}$	$x+2x^2+2x^3+2x^4+x^5$
$\Gamma_4$	$T_{31}-iT_{23}$ $P_1+iP_2$	$G_{31}-iG_{23}$	$x+2x^2+2x^3+2x^4+x^5$

I.R.	Canonical Expressions
$\Gamma_1$	$a_0 + \sum_{i=1}^6 a_i L_i + a_7 L_1 L_2$
$\Gamma_2$	$\sum_{i=1}^4 b_i J_i + b_5 L_1 J_1 + b_6 L_2 J_2 + b_7 L_1 J_4 + b_8 L_2 J_3$
$\Gamma_3$	$\sum_{i=1}^4 c_i R_i + c_5 L_1 R_1 + c_6 L_2 R_1 + c_7 L_2 R_2 + c_8 L_3 R_1$
$\Gamma_4$	$\sum_{i=1}^4 \bar{c}_i \bar{R}_i + \bar{c}_5 L_1 \bar{R}_1 + \bar{c}_6 L_2 \bar{R}_1 + \bar{c}_7 L_2 \bar{R}_2 + \bar{c}_8 L_3 \bar{R}_1$

Table 3.18 Tetragonal-pyramidal class,  $C_4$

I.R.	Basic Quantities		$Z_v$
$\Gamma_1$	$T_{11}+T_{22}, T_{33}$ $P_3$	$G_{11}+G_{22}, G_{33}$	$1+x^2+4x^3+x^4+x^6$
$\Gamma_2$	$T_{11}-T_{22}, T_{12}$	$G_{11}-G_{22}, G_{12}$	$2(x+x^2+x^4+x^5)$
$\Gamma_3$	$T_{31}+iT_{23}$ $P_1+iP_2$	$G_{31}+iG_{23}$	$x+2x^2+2x^3+2x^4+x^5$
$\Gamma_4$	$T_{31}-iT_{23}$ $P_1-iP_2$	$G_{31}-iG_{23}$	$x+2x^2+2x^3+2x^4+x^5$

I.R.	Canonical Expressions
$\Gamma_1$	$a_0 + \sum_{i=1}^6 a_i L_i + a_7 L_1 L_2$
$\Gamma_2$	$\sum_{i=1}^4 b_i J_i + b_5 L_1 J_1 + b_6 L_2 J_2 + b_7 L_1 J_4 + b_8 L_2 J_3$
$\Gamma_3$	$\sum_{i=1}^4 c_i R_i + c_5 L_1 R_1 + c_6 L_2 R_1 + c_7 L_2 R_2 + c_8 L_3 R_1$
$\Gamma_4$	$\sum_{i=1}^4 \bar{c}_i \bar{R}_i + \bar{c}_5 L_1 \bar{R}_1 + \bar{c}_6 L_2 \bar{R}_1 + \bar{c}_7 L_2 \bar{R}_2 + \bar{c}_8 L_3 \bar{R}_1$

Table 3.19 Tetragonal-dipyramidal class,  $C_{4h}$

I.R.	Basic Quantities		$Z_v$
$\Gamma_1$	$T_{11}+T_{22}, T_{33}$	$G_{11}+G_{22}, G_{33}$	$1+x^2+4x^3+x^4+x^6$
$\Gamma_2$	$T_{11}-T_{22}, T_{12}$	$G_{11}-G_{22}, G_{12}$	$2(x+x^2+x^4+x^5)$
$\Gamma_3$	$T_{31}+iT_{23}$	$G_{23}+iG_{23}$	$x+2x^2+2x^3+2x^4+x^5$
$\Gamma_4$	$T_{31}-iT_{23}$	$G_{31}-iG_{23}$	$x+2x^2+2x^3+2x^4+x^5$
$\Gamma_5$	$P_3$		0
$\Gamma_6$			0
$\Gamma_7$	$P_1+iP_2$		0
$\Gamma_8$	$P_1-iP_2$		0

I.R.	Canonical Expressions
$\Gamma_1$	$a_0 + \sum_{i=1}^6 a_i L_i + a_7 L_1 L_2$
$\Gamma_2$	$\sum_{i=1}^4 b_i J_i + b_5 L_1 J_1 + b_6 L_2 J_2 + b_7 L_1 J_4 + b_8 L_2 J_3$
$\Gamma_3$	$\sum_{i=1}^4 c_i R_i + c_5 L_1 R_1 + c_6 L_2 R_1 + c_7 L_2 R_2 + c_8 L_3 R_1$
$\Gamma_4$	$\sum_{i=1}^4 \bar{c}_i \bar{R}_i + \bar{c}_5 L_1 \bar{R}_1 + \bar{c}_6 L_2 \bar{R}_1 + \bar{c}_7 L_2 \bar{R}_2 + \bar{c}_8 L_3 \bar{R}_1$
$\Gamma_5$	None
$\Gamma_6$	None
$\Gamma_7$	None
$\Gamma_8$	None



Integrity Basis:  $S_4, C_4, C_{4h}$

$$K_1, \dots, K_6 = G_{11} + G_{22}, G_{11}G_{22}, G_{33}, G_{23}^2 + G_{31}^2, G_{23}^2G_{31}^2, G_{12}^2$$

$$L_1 = G_{23}G_{31}G_{12}, L_2 = (G_{11}-G_{22})(G_{31}^2-G_{12}^2), L_3 = G_{12}(G_{11}-G_{22}),$$

$$L_4 = G_{12}(G_{31}^2-G_{23}^2), L_5 = G_{23}G_{31}(G_{11}-G_{22}), L_6 = G_{23}G_{31}(G_{31}^2-G_{23}^2)$$

Quantities of type  $\Gamma_2$  appearing in Tables 3.17, 3.18, 3.19

$$J_1 = G_{11}-G_{22}, J_2 = G_{12}, J_3 = G_{23}G_{31}, J_4 = G_{31}^2-G_{23}^2$$

Quantities of type  $\Gamma_3$  appearing in Tables 3.17, 3.18, 3.19

$$R_1 = G_{31}+iG_{23}, R_2 = G_{12}(G_{31}-iG_{23}), R_3 = (G_{11}-G_{22})(G_{31}-iG_{23}),$$

$$R_4 = G_{23}G_{31}(G_{31}-iG_{23})$$

Generating Function:  $S_4, C_4, C_{4h}$

$$GF(\Gamma_v) = \frac{Z_v}{(1-x)^2(1-x^2)^3(1-x^4)}$$

In table 3.17, the quantities  $c_0, \dots, c_8$  appearing in the columns headed Canonical Expressions are polynomial functions of the invariants  $K_1, \dots, K_6$  where the coefficients in the expressions for  $c_1, \dots, c_8$  are complex numbers. Thus,

$$c_1 = (\alpha_1+i\alpha_2) + (\beta_1+i\beta_2)K_1 + (\gamma_1+i\gamma_2)K_2 + \dots$$

The coefficients  $\bar{c}_0, \dots, \bar{c}_8$  and the quantities  $\bar{R}_1, \dots, \bar{R}_4$  are the complex conjugates of the coefficients  $c_0, \dots, c_8$  and the quantities  $R_1, \dots, R_4$  respectively. Thus,

$$\bar{C}_1 = (\alpha_1 - i\alpha_2) + (\beta_1 - i\beta_2)K_1 + (\gamma_1 - i\gamma_2)K_2 + \dots$$

$$\bar{R}_1 = G_{31} - iG_{23}, \dots, \bar{R}_4 = G_{23}G_{31}(G_{31} + iG_{23})$$

We note that the expressions for the complex quantities such as  $T_{31} + iT_{23}$  and  $T_{31} - iT_{23}$  which are of types  $\Gamma_3$  and  $\Gamma_4$  respectively may also be written in real form. For example, we see from Table 3.17 that for the crystal class  $S_4$

$$\begin{aligned} T_{31} + iT_{23} = & (\alpha_1 + i\alpha_2)(G_{31} + iG_{23}) + (\beta_1 + i\beta_2)K(G_{31} + iG_{23}) + \dots \\ & + (\alpha'_1 + i\alpha'_2)L_3(G_{31} + iG_{23}) + (\beta'_1 + i\beta'_2)K_1L_3(G_{31} + iG_{23}) + \dots \end{aligned}$$

Upon separating the real and imaginary parts of this expression, we obtain

$$\begin{aligned} \begin{vmatrix} T_{31} \\ T_{23} \end{vmatrix} = & \begin{vmatrix} \alpha_1 & -\alpha_2 \\ \alpha_2 & \alpha_1 \end{vmatrix} \begin{vmatrix} G_{31} \\ G_{23} \end{vmatrix} + \begin{vmatrix} \beta_1 & -\beta_2 \\ \beta_2 & \beta_1 \end{vmatrix} \begin{vmatrix} K_1G_{31} \\ K_1G_{23} \end{vmatrix} + \dots \\ & + \begin{vmatrix} \alpha'_1 & -\alpha'_2 \\ \alpha'_2 & \alpha'_1 \end{vmatrix} \begin{vmatrix} L_3G_{31} \\ L_3G_{23} \end{vmatrix} + \begin{vmatrix} \beta'_1 & -\beta'_2 \\ \beta'_2 & \beta'_1 \end{vmatrix} \begin{vmatrix} K_1L_3G_{31} \\ K_1L_3G_{23} \end{vmatrix} + \dots \end{aligned}$$

The real form given above may be more convenient in applications.

3.3.6 Ditetragonal-pyramidal class,  $C_{4v}, (\underline{I}, \underline{R}_1, \underline{R}_2, \underline{D}_3) \cdot (\underline{I}, \underline{T}_3)$

Tetragonal-trapezohedral class,  $D_4, (\underline{I}, \underline{D}_1, \underline{D}_2, \underline{D}_3, \underline{CT}_3, \underline{R}_1 \underline{T}_3, \underline{R}_2 \underline{T}_3, \underline{R}_3 \underline{T}_3)$

Tetragonal-scalenohedral class,  $D_{2d}, (\underline{I}, \underline{D}_1, \underline{D}_2, \underline{D}_3) \cdot (\underline{I}, \underline{T}_3)$

Ditetragonal-dipyramidal class,  $D_{4h}, (\underline{I}, \underline{C}, \underline{R}_1, \underline{R}_2, \underline{R}_3, \underline{D}_1, \underline{D}_2, \underline{D}_3) \cdot (\underline{I}, \underline{T}_3)$

Table 3.20 Irreducible Representations:  $C_{4v}, D_4, D_{2d}$

	$\underline{I}$	$\underline{R}_2$	$\underline{R}_1$	$\underline{D}_3$	$\underline{T}_3$	$\underline{R}_2 \underline{T}_3$	$\underline{R}_1 \underline{T}_3$	$\underline{D}_3 \underline{T}_3$
$C_4$	$\underline{I}$	$\underline{R}_2$	$\underline{R}_1$	$\underline{D}_3$	$\underline{T}_3$	$\underline{R}_2 \underline{T}_3$	$\underline{R}_1 \underline{T}_3$	$\underline{D}_3 \underline{T}_3$
$D_4$	$\underline{I}$	$\underline{D}_1$	$\underline{D}_2$	$\underline{D}_3$	$\underline{R}_3 \underline{T}_3$	$\underline{R}_2 \underline{T}_3$	$\underline{R}_1 \underline{T}_3$	$\underline{CT}_3$
$D_{2d}$	$\underline{I}$	$\underline{D}_1$	$\underline{D}_2$	$\underline{D}_3$	$\underline{T}_3$	$\underline{D}_1 \underline{T}_3$	$\underline{D}_2 \underline{T}_3$	$\underline{D}_3 \underline{T}_3$
$\Gamma_1$	1	1	1	1	1	1	1	1
$\Gamma_2$	1	-1	-1	1	-1	1	1	-1
$\Gamma_3$	1	-1	-1	1	1	-1	-1	1
$\Gamma_4$	1	1	1	1	-1	-1	-1	-1
$\Gamma_5$	$\underline{E}$	$\underline{F}$	$-\underline{F}$	$-\underline{E}$	$\underline{K}$	$\underline{L}$	$-\underline{L}$	$-\underline{K}$

Table 3.21 Irreducible Representations,  $D_{4h}$

$D_{4h}$	$\Gamma$	$D_1$	$D_2$	$D_3$	$\Gamma_1$	$R_1\Gamma_3$	$R_2\Gamma_3$	$R_3\Gamma_3$
$\Gamma_1$	1	1	1	1	1	1	1	1
$\Gamma_2$	1	-1	-1	1	1	1	1	-1
$\Gamma_3$	1	-1	-1	1	1	-1	-1	1
$\Gamma_4$	1	1	1	1	-1	-1	-1	-1
$\Gamma_5$	$\tilde{E}$	$\tilde{F}$	$-\tilde{F}$	$-\tilde{E}$	$-\tilde{K}$	$-\tilde{L}$	$\tilde{L}$	$\tilde{K}$
$\Gamma_6$	1	1	1	1	1	1	1	1
$\Gamma_7$	1	-1	-1	1	-1	1	1	-1
$\Gamma_8$	1	-1	-1	1	1	-1	-1	1
$\Gamma_9$	1	1	1	1	-1	-1	-1	-1
$\Gamma_{10}$	$\tilde{E}$	$\tilde{F}$	$-\tilde{F}$	$-\tilde{E}$	$-\tilde{K}$	$-\tilde{L}$	$\tilde{L}$	$\tilde{K}$

$D_{4h}$	$C$	$R_1$	$R_2$	$R_3$	$\Gamma_3$	$D_1\Gamma_3$	$D_2\Gamma_3$	$D_3\Gamma_3$
$\Gamma_1$	1	1	1	1	1	1	1	1
$\Gamma_2$	1	-1	-1	1	-1	1	1	-1
$\Gamma_3$	1	-1	-1	1	1	-1	-1	1
$\Gamma_4$	1	1	1	1	-1	-1	-1	-1
$\Gamma_5$	$\tilde{E}$	$\tilde{F}$	$-\tilde{F}$	$-\tilde{E}$	$-\tilde{K}$	$-\tilde{L}$	$\tilde{L}$	$\tilde{K}$
$\Gamma_6$	-1	-1	-1	-1	-1	-1	-1	-1
$\Gamma_7$	-1	1	1	-1	1	-1	-1	1
$\Gamma_8$	-1	1	1	-1	-1	1	1	-1
$\Gamma_9$	-1	-1	-1	-1	1	1	1	1
$\Gamma_{10}$	$-\tilde{E}$	$-\tilde{F}$	$\tilde{F}$	$\tilde{E}$	$\tilde{K}$	$\tilde{L}$	$-\tilde{L}$	$-\tilde{K}$

In Tables 3.20 and 3.21, we have employed the notation

$$\tilde{E} = \begin{vmatrix} 1 & 0 \\ 0 & 1 \end{vmatrix}, \tilde{F} = \begin{vmatrix} 1 & 0 \\ 0 & -1 \end{vmatrix}, \tilde{K} = \begin{vmatrix} 0 & 1 \\ 1 & 0 \end{vmatrix}, \tilde{L} = \begin{vmatrix} 0 & 1 \\ -1 & 0 \end{vmatrix}.$$

Table 3.22 Ditetragonal-pyramidal class,  $C_{4v}$

I.R.	Basic Quantities		$Z_v$
$\Gamma_1$	$T_{11}+T_{22}, T_{33}$ $P_3$	$G_{11}+G_{22}, G_{33}$	$1 + 2x^3 + x^6$
$\Gamma_2$			$x^2 + 2x^3 + x^4$
$\Gamma_3$	$T_{12}$	$G_{12}$	$x + x^2 + x^4 + x^5$
$\Gamma_4$	$T_{11}-T_{22}$	$G_{11}-G_{22}$	$x + x^2 + x^4 + x^5$
$\Gamma_5$	$(T_{31}, T_{23})^T$ $(P_1, P_2)^T$	$(G_{31}, G_{23})^T$	$x + 2x^2 + 2x^3 + 2x^4 + x^5$
I.R.	Canonical Expressions		
$\Gamma_1$	$a_0 + a_1 L_1 + a_2 L_2 + a_3 L_1 L_2$		
$\Gamma_2$	$\sum_{i=1}^4 b_i M_i$		
$\Gamma_3$	$c_1 I_1 + c_2 I_2 + c_3 L_2 I_1 + c_4 L_2 I_2$		
$\Gamma_4$	$d_1 J_1 + d_2 J_2 + d_3 L_1 J_1 + d_4 L_1 J_2$		
$\Gamma_5$	$\sum_{i=1}^5 e_i N_i + e_6 L_1 N_1 + e_7 L_1 N_3 + e_8 L_2 N_1$		

Table 3.23 Tetragonal-trapezohedral class,  $D_4$

I.R.	Basic Quantities		$Z_v$
$\Gamma_1$	$T_{11}+T_{22}, T_{33}$	$G_{11}+G_{22}, G_{33}$	$1 + 2x^3 + x^6$
$\Gamma_2$	$P_3$		$x^2 + 2x^3 + x^4$
$\Gamma_3$	$T_{12}$	$G_{12}$	$x + x^2 + x^4 + x^5$
$\Gamma_4$	$T_{11}-T_{22}$	$G_{11}-G_{22}$	$x + x^2 + x^4 + x^5$
$\Gamma_5$	$(T_{23}, -T_{31})^T$ $(P_1, P_2)^T$	$(G_{23}, -G_{31})^T$	$x + 2x^2 + 2x^3 + 2x^4 + x^5$

I.R.	Canonical Expressions
$\Gamma_1$	$a_0 + a_1 L_1 + a_2 L_2 + a_3 L_1 L_2$
$\Gamma_2$	$\sum_{i=1}^4 b_i M_i$
$\Gamma_3$	$c_1 I_1 + c_2 I_2 + c_3 L_2 I_1 + c_4 L_2 I_2$
$\Gamma_4$	$d_1 J_1 + d_2 J_2 + d_3 L_1 J_1 + d_4 L_1 J_2$
$\Gamma_5$	$\sum_{i=1}^5 e_i Q_i + e_6 L_1 Q_1 + e_7 L_1 Q_3 + e_8 L_2 Q_1$

Table 3.24 Tetragonal-scalenohedral class,  $D_{2d}$

I.R.	Basic Quantities		$Z_v$
$\Gamma_1$	$T_{11}+T_{22}, T_{33}$	$G_{11}+G_{22}, G_{33}$	$1 + 2x^3 + x^6$
$\Gamma_2$			$x^2 + 2x^3 + x^4$
$\Gamma_3$	$T_{12}; P_3$	$G_{12}$	$x + x^2 + x^4 + x^5$
$\Gamma_4$	$T_{11}-T_{22}$	$G_{11}-G_{22}$	$x + x^2 + x^4 + x^5$
$\Gamma_5$	$(T_{23}, T_{31})^T$ $(P_1, P_2)^T$	$(G_{23}, G_{31})^T$	$x + 2x^2 + 2x^3 + 2x^4 + x^5$

I.R.	Canonical Expressions
$\Gamma_1$	$a_0 + a_1 L_1 + a_2 L_2 + a_3 L_1 L_2$
$\Gamma_2$	$\sum_{i=1}^4 b_i M_i$
$\Gamma_3$	$c_1 I_1 + c_2 I_2 + c_3 L_2 I_1 + c_4 L_2 I_2$
$\Gamma_4$	$d_1 J_1 + d_2 J_2 + d_3 L_1 J_1 + d_4 L_1 J_2$
$\Gamma_5$	$\sum_{i=1}^5 e_i R_i + e_6 L_1 R_1 + e_7 L_1 R_3 + e_8 L_2 R_1$

Table 3.25 Ditetragonal-dipyramidal class,  $D_{4h}$

I.R.	Basic Quantities		$Z_v$
$\Gamma_1$	$T_{11}+T_{22}, T_{33}$	$G_{11}+G_{22}, G_{33}$	$1 + 2x^3 + x^6$
$\Gamma_3$	$T_{12}$	$G_{12}$	$x + x^2 + x^4 + x^5$
$\Gamma_4$	$T_{11}-T_{22}$	$G_{11}-G_{22}$	$x + x^2 + x^4 + x^5$
$\Gamma_5$	$(T_{23}, -T_{31})^T$	$(G_{23}, -G_{31})^T$	$x + 2x^2 + 2x^3 + 2x^4 + x^5$
$\Gamma_7$	$P_3$		0
$\Gamma_{10}$	$(P_1, P_2)^T$		0

I.R.	Canonical Expressions
$\Gamma_1$	$a_0 + a_1 L_1 + a_2 L_2 + a_3 L_1 L_2$
$\Gamma_3$	$c_1 I_1 + c_2 I_2 + c_3 L_2 I_1 + c_4 L_2 I_2$
$\Gamma_4$	$d_1 J_1 + d_2 J_2 + d_3 L_1 J_1 + d_4 L_1 J_2$
$\Gamma_5$	$\sum_{i=1}^5 e_i Q_i + e_6 L_1 Q_1 + e_7 L_1 Q_3 + e_8 L_2 Q_1$
$\Gamma_7$	None
$\Gamma_{10}$	None



Integrity Basis:  $C_{4v}$ ,  $d_4$ ,  $D_{2d}$ ,  $D_{4h}$

$$K_1, \dots, K_6 = G_{11} + G_{22}, G_{11}G_{22}, G_{33}, G_{23}^2 + G_{31}^2, G_{31}^2G_{23}^2, G_{12}^2$$

$$L_1 = G_{23}G_{31}G_{12}, L_2 = (G_{11}-G_{22})(G_{31}^2-G_{23}^2)$$

Quantities of type  $\Gamma_2$  appearing in Tables 3.22, ..., 3.25

$$M_1 = G_{12}(G_{11}-G_{22}), M_2 = G_{12}(G_{31}^2-G_{23}^2), M_3 = G_{23}G_{31}(G_{11}-G_{22}),$$

$$M_4 = G_{23}G_{31}(G_{31}^2-G_{23}^2)$$

Quantities of type  $\Gamma_3$  appearing in Tables 3.22, ..., 3.25

$$I_1 = G_{12}, I_2 = G_{23}G_{31}$$

Quantities of type  $\Gamma_4$  appearing in Tables 3.22, ..., 3.25

$$J_1 = G_{11}-G_{22}, J_2 = G_{31}^2-G_{23}^2$$

Quantities of type  $\Gamma_5$  appearing in Tables 3.22, ..., 3.25

$$\tilde{N}_1 = \begin{vmatrix} G_{31} \\ G_{23} \end{vmatrix}, \tilde{N}_2 = G_{12} \begin{vmatrix} G_{23} \\ G_{31} \end{vmatrix}, \tilde{N}_3 = (G_{11}-G_{22}) \begin{vmatrix} G_{31} \\ -G_{23} \end{vmatrix},$$

$$\tilde{N}_4 = G_{12}(G_{11}-G_{22}) \begin{vmatrix} G_{23} \\ -G_{31} \end{vmatrix}, \tilde{N}_5 = G_{23}G_{31} \begin{vmatrix} G_{23} \\ G_{31} \end{vmatrix},$$

$$\tilde{Q}_1 = \begin{vmatrix} G_{23} \\ -G_{31} \end{vmatrix}, \tilde{Q}_2 = G_{12} \begin{vmatrix} -G_{31} \\ G_{23} \end{vmatrix}, \tilde{Q}_3 = (G_{11}-G_{22}) \begin{vmatrix} G_{23} \\ G_{31} \end{vmatrix},$$

$$\tilde{Q}_4 = G_{12}(G_{11}-G_{22}) \begin{vmatrix} G_{31} \\ G_{23} \end{vmatrix}, \tilde{Q}_5 = G_{23}G_{31} \begin{vmatrix} -G_{31} \\ G_{23} \end{vmatrix},$$

$$\tilde{R}_1 = \begin{vmatrix} G_{23} \\ G_{31} \end{vmatrix}, \quad \tilde{R}_2 = G_{12} \begin{vmatrix} G_{31} \\ G_{23} \end{vmatrix}, \quad \tilde{R}_3 = (G_{11} - G_{22}) \begin{vmatrix} G_{23} \\ G_{31} \end{vmatrix},$$

$$\tilde{R}_4 = G_{12}(G_{11} - G_{22}) \begin{vmatrix} G_{31} \\ -G_{23} \end{vmatrix}, \quad \tilde{R}_5 = G_{23}G_{31} \begin{vmatrix} G_{31} \\ G_{23} \end{vmatrix}$$

Generating Function:  $C_{4v}, D_4, D_{2d}, D_{4h}$

$$GF(\Gamma_v) = \frac{Z_v}{(1-x)^2(1-x^2)^3(1-x^4)}$$

### 3.3.7 Trigonal-pyramidal class, $C_3$ , ( $I, S_1, S_2$ )

Table 3.26 Irreducible Representations:  $C_3$

$C_3$	$I$	$S_1$	$S_2$
$\Gamma_1$	1	1	1
$\Gamma_2$	1	$\omega$	$\omega^2$
$\Gamma_3$	1	$\omega^2$	$\omega$

Table 3.27 Rhombohedral class:  $C_{3i}$

$C_{3i}$	$I$	$S_1$	$S_2$	$C$	$CS_1$	$CS_2$
$\Gamma_1$	1	1	1	1	1	1
$\Gamma_2$	1	$\omega$	$\omega^2$	1	$\omega$	$\omega^2$
$\Gamma_3$	1	$\omega^2$	$\omega$	1	$\omega^2$	$\omega$
$\Gamma_4$	1	1	1	-1	-1	-1
$\Gamma_5$	1	$\omega$	$\omega^2$	-1	$-\omega$	$-\omega^2$
$\Gamma_6$	1	$\omega^2$	$\omega$	-1	$-\omega^2$	$-\omega$

The quantities  $\omega$  and  $\omega^2$  appearing in Tables 3.26 and 3.27 are defined by

$$\omega = -1/2 + i\sqrt{3}/2, \quad \omega^2 = -1/2 - i\sqrt{3}/2.$$

Table 3.28 Trigonal-pyramidal class,  $C_3$

I.R.	Basic Quantities		$Z_v$
$\Gamma_1$	$T_{11}+T_{22}, T_{33}$ $P_3$	$G_{11}+G_{22}, G_{33}$	$1 + 2x^2 + 6x^3 + 2x^4 + x^6$
$\Gamma_2$	$T_{31}-iT_{23}$ $T_{11}-T_{22}+2iT_{12}$ $P_1-iP_2$	$G_{31}-iG_{23}$ $G_{11}-G_{22}+2iG_{12}$	$2x + 3x^2 + 2x^3 + 3x^4 + 2x^5$
$\Gamma_3$	$T_{31}+iT_{23}$ $T_{11}-T_{22}-2iT_{12}$ $P_1+iP_2$	$G_{31}+iG_{23}$ $G_{11}-G_{22}-2iG_{12}$	$2x + 3x^2 + 2x^3 + 3x^4 + 2x^5$

I.R.	Canonical Expressions
$\Gamma_1$	$a_0 + \sum_{i=1}^8 a_i L_i + a_9 L_1^2 + a_{10} L_2 L_3 + a_{11} L_1 L_4$
$\Gamma_2$	$\sum_{i=1}^5 b_i J_i + (b_6 L_1 + b_7 L_2 + b_8 L_3) J_1 + (b_9 L_1 + b_{10} L_2) J_2$ $+ b_{11} L_6 J_3 + b_{12} L_5 J_4$
$\Gamma_3$	$\sum_{i=1}^5 \bar{b}_i \bar{J}_i + (\bar{b}_6 L_1 + \bar{b}_7 L_2 + \bar{b}_8 L_3) \bar{J}_1 + (\bar{b}_9 L_1 + \bar{b}_{10} L_2) \bar{J}_2$ $+ \bar{b}_{11} L_6 \bar{J}_3 + \bar{b}_{12} L_5 \bar{J}_4$

Table 3.29 Rhombohedral class,  $C_{3i}$

I.R.	Basic Quantities		$Z_v$
$\Gamma_1$	$T_{11}+T_{22}, T_{33}$	$G_{11}+G_{22}, G_{33}$	$1 + 2x^2 + 6x^3 + 2x^4 + x^6$
$\Gamma_2$	$T_{31}-iT_{23}$	$G_{31}-iG_{23}$	$2x + 3x^2 + 2x^3 + 3x^4 + 2x^5$
	$T_{11}-T_{22}+2iT_{12}$	$G_{11}-G_{22}+2iG_{12}$	
$\Gamma_3$	$T_{31}+iT_{23}$	$G_{31}+iG_{23}$	$2x + 3x^2 + 2x^3 + 3x^4 + 2x^5$
	$T_{11}-T_{22}-2iT_{12}$	$G_{11}-G_{22}-2iG_{12}$	
$\Gamma_4$	$P_3$		0
$\Gamma_5$	$P_1-iP_2$		0
$\Gamma_6$	$P_1+iP_2$		0

I.R.	Canonical Expressions
$\Gamma_1$	$a_0 + \sum_{i=1}^8 a_i L_i + a_9 L_1^2 + a_{10} L_2 L_3 + a_{11} L_1 L_4$
$\Gamma_2$	$\sum_{i=1}^5 b_i J_i + (b_6 L_1 + b_7 L_2 + b_8 L_3) J_1 + (b_9 L_1 + b_{10} L_2) J_2 + b_{11} L_6 J_3 + b_{12} L_5 J_4$
$\Gamma_3$	$\sum \bar{b}_i \bar{J}_i + (\bar{b}_6 L_1 + \bar{b}_7 L_2 + \bar{b}_8 L_3) \bar{J}_1 + (\bar{b}_9 L_1 + \bar{b}_{10} L_2) \bar{J}_2 + \bar{b}_{11} L_6 \bar{J}_3 + \bar{b}_{12} L_5 \bar{J}_4$
$\Gamma_4$	None
$\Gamma_5$	None
$\Gamma_6$	None

We employ below the notation

$$g = G_{31} - iG_{23}, \quad \bar{g} = G_{31} + iG_{23}, \quad G = G_{11} - G_{22} + 2iG_{12},$$

$$\bar{G} = G_{11} - G_{22} - 2iG_{12}.$$

Integrity Basis:  $C_3, C_{3i}$

$$K_1, \dots, K_6 = G_{11} + G_{22}, G\bar{G}, G^3 + \bar{G}^3, G_{33}, g\bar{g}, g^3 - \bar{g}^3,$$

$$L_1 = g\bar{G} - \bar{g}G, \quad L_2 = g^2G + \bar{g}^2\bar{G}, \quad L_3 = \bar{g}\bar{G}^2 - gG^2, \quad L_4 = g\bar{G} + \bar{g}G,$$

$$L_5 = G^3 - \bar{G}^3, \quad L_6 = g^3 + \bar{g}^3, \quad L_7 = gG^2 + \bar{g}\bar{G}^2, \quad L_8 = g^2G - \bar{g}^2\bar{G}$$

Quantities of type  $\Gamma_2$  appearing in Tables 3.28 and 3.29

$$J_1, \dots, J_5 = G, g, \bar{G}^2, \bar{g}^2, g\bar{G}$$

Quantities of type  $\Gamma_3$  appearing in Tables 3.28 and 3.29

$$\bar{J}_1, \dots, \bar{J}_5 = \bar{G}, \bar{g}, G^2, g^2, gG$$

The coefficients  $b_1, \dots, b_{12}$  appearing in Table 3.28 are polynomial functions of the invariants  $K_1, \dots, K_6$  where the coefficients in the expressions for  $b_1, \dots, b_{12}$  are complex numbers. Thus,

$$b_1 = (\alpha_1 + i\alpha_2) + (\beta_1 + i\beta_2)K_1 + (\gamma_1 + i\gamma_2)K_2 + \dots$$

and

$$\bar{b}_1 = (\alpha_1 - i\alpha_2) + (\beta_1 - i\beta_2)K_1 + (\gamma_1 - i\gamma_2)K_2 + \dots$$

Generating Function:  $C_3, C_{3i}$

$$GF(\Gamma_v) = \frac{Z_v}{(1-x)^2(1-x^2)^2(1-x^3)^2}$$

3.3.8 Ditrigonal-pyramidal class,  $C_{3v}, (\underline{I}, \underline{R}_1) \cdot (\underline{I}, \underline{S}_1, \underline{S}_2)$

Trigonal-trapezohedral class,  $D_3, (\underline{I}, \underline{D}_1) \cdot (\underline{I}, \underline{S}_1, \underline{S}_2)$

Table 3.30 Irreducible Representations:  $C_{3v}, D_3$

$C_{3v}$	$\underline{I}$	$\underline{S}_1$	$\underline{S}_2$	$\underline{R}_1$	$\underline{R}_1 \underline{S}_1$	$\underline{R}_1 \underline{S}_2$
$D_3$	$\underline{I}$	$\underline{S}_1$	$\underline{S}_2$	$\underline{D}_1$	$\underline{D}_1 \underline{S}_1$	$\underline{D}_1 \underline{S}_2$
$\Gamma_1$	1	1	1	1	1	1
$\Gamma_2$	1	1	1	-1	-1	-1
$\Gamma_3$	$\underline{E}$	$\underline{A}$	$\underline{B}$	$-\underline{F}$	$-\underline{G}$	$-\underline{H}$

In Table 3.30, we have employed the notation

$$\underline{E} = \begin{vmatrix} 1 & 0 \\ 0 & 1 \end{vmatrix}, \quad \underline{A} = \begin{vmatrix} -1/2 & \sqrt{3}/2 \\ -\sqrt{3}/2 & -1/2 \end{vmatrix}, \quad \underline{B} = \begin{vmatrix} -1/2 & -\sqrt{3}/2 \\ \sqrt{3}/2 & -1/2 \end{vmatrix},$$

$$\underline{F} = \begin{vmatrix} 1 & 0 \\ 0 & -1 \end{vmatrix}, \quad \underline{G} = \begin{vmatrix} -1/2 & \sqrt{3}/2 \\ \sqrt{3}/2 & 1/2 \end{vmatrix}, \quad \underline{H} = \begin{vmatrix} -1/2 & -\sqrt{3}/2 \\ -\sqrt{3}/2 & 1/2 \end{vmatrix}.$$

Table 3.31 Ditrigonal-pyramidal class,  $C_{3v}$

I.R.	Basic Quantities		$Z_v$
$\Gamma_1$	$T_{11}+T_{22}, T_{33}$ $P_3$	$G_{11}+G_{22}, G_{33}$	$1+x^2+2x^3+x^4+x^6$
$\Gamma_2$			$x^2+4x^3+x^4$
$\Gamma_3$	$(T_{31}, T_{23})^T$ $(2T_{12}, T_{11}-T_{22})^T$ $(P_1, P_2)^T$	$(G_{31}, G_{23})^T$ $(2G_{12}, G_{11}-G_{22})^T$	$2x+3x^2+2x^3+3x^4+2x^5$

I.R.	Canonical Expressions
$\Gamma_1$	$a_0 + a_1 L_1 + a_2 L_2 + a_3 L_3 + a_4 L_1^2 + a_5 L_2 L_3$
$\Gamma_2$	$\sum_{i=1}^5 b_i M_i + b_6 L_1 M_1$
$\Gamma_3$	$\sum_{i=1}^5 c_i J_i + (c_6 L_1 + c_7 L_2) J_1 + (c_8 L_1 + c_9 L_2) J_2 + (c_{10} L_1 + c_{11} L_2) J_3 +$ $+ c_{12} L_3 J_4$



Table 3.32 Trigonal-trapezohedral class,  $D_3$

I.R.	Basic Quantities		$Z_v$
$\Gamma_1$	$T_{11}+T_{22}, T_{33}$	$G_{11}+G_{22}, G_{33}$	$1+x^2+2x^3+x^4+x^6$
$\Gamma_2$	$P_3$		$x^2+4x^3+x^4$
$\Gamma_3$	$(T_{31}, T_{23})^T$ $(2T_{12}, T_{11}-T_{22})^T$ $(P_2, -P_1)^T$	$(G_{31}, G_{23})^T$ $(2G_{12}, G_{11}-G_{22})^T$	$2x+3x^2+2x^3+3x^4+2x^5$

I.R.	Canonical Expressions
$\Gamma_1$	$a_0 + a_1 L_1 + a_2 L_2 + a_3 L_3 + a_4 L_1^2 + a_5 L_2 L_3$
$\Gamma_2$	$\sum_{i=1}^5 b_i M_i + b_6 L_1 M_1$
$\Gamma_3$	$\sum_{i=1}^5 c_i J_i + (c_6 L_1 + c_7 L_2) J_1 + (c_8 L_1 + c_9 L_2) J_2 + (c_{10} L_1 + c_{11} L_2) J_3 + c_{12} L_3 J_4$

Integrity Basis:  $C_{3v}, D_3$

$$K_1, \dots, K_3 = G_{11}+G_{22}, (G_{11}-G_{22})+4G_{12}^2, (G_{11}-G_{22})^3 - 12(G_{11}-G_{22})G_{12}^2$$

$$K_4, \dots, K_6 = G_{33}, G_{31}^2 + G_{23}^2, G_{23}^3 - 3G_{23}G_{31}^2$$

$$L_1 = (G_{11}-G_{12})G_{23} + 2G_{31}G_{12}, L_2 = (G_{11}-G_{22})(G_{31}^2 - G_{23}^2) + 4G_{12}G_{23}G_{31},$$

$$L_3 = (G_{11}-G_{22})^2 G_{23} - 4G_{12}^2 G_{23} - 4(G_{11}-G_{22})G_{12}G_{31}$$

Quantities of type  $\Gamma_2$  appearing in Tables 3.31 and 3.32

$$\begin{aligned}
M_1 &= (G_{11}-G_{22})G_{31}-2G_{12}G_{23} , \quad M_2 = 3(G_{11}-G_{22})^2G_{12}-4G_{12}^3 , \\
M_3 &= G_{31}^3-3G_{31}G_{23}^2 , \quad M_4 = (G_{11}-G_{22})^2G_{31}-4G_{12}^2G_{31}+4(G_{11}-G_{22})G_{12}G_{23} , \\
M_5 &= (G_{11}-G_{22})G_{23}G_{31}-G_{12}(G_{31}^2-G_{23}^2)
\end{aligned}$$

Quantities of type  $\Gamma_3$  appearing in Tables 3.31 and 3.32

$$\begin{aligned}
J_1 &= \left\| \begin{array}{c} 2G_{12} \\ G_{11}-G_{22} \end{array} \right\| , \quad J_2 = \left\| \begin{array}{c} G_{31} \\ G_{23} \end{array} \right\| , \quad J_3 = \left\| \begin{array}{c} -4(G_{11}-G_{22})G_{12} \\ (G_{11}-G_{22})^2-4G_{12}^2 \end{array} \right\| , \\
J_4 &= \left\| \begin{array}{c} 2G_{23}G_{31} \\ G_{31}^2-G_{23}^2 \end{array} \right\| , \quad J_5 = \left\| \begin{array}{c} (G_{11}-G_{22})G_{31} + 2G_{12}G_{23} \\ -(G_{11}-G_{22})G_{23} + 2G_{12}G_{31} \end{array} \right\|
\end{aligned}$$

Generating Function:  $C_{3v}$  ,  $D_3$

$$GF(\Gamma_v) = \frac{Z_v}{(1-x)^2(1-x^2)^2(1-x^3)^2}$$

3.3.9 Trigonal-dipyramidal class,  $C_{3h}, (\underline{I}, \underline{R}_3) \cdot (\underline{I}, \underline{S}_1, \underline{S}_2)$

Hexagonal-pyramidal class,  $C_6, (\underline{I}, \underline{D}_3) \cdot (\underline{I}, \underline{S}_1, \underline{S}_2)$

Table 3.33 Irreducible Representations:  $C_{3h}, C_6$

$C_{3h}$	$\underline{I}$	$\underline{S}_1$	$\underline{S}_2$	$\underline{R}_3$	$\underline{R}_3 \underline{S}_1$	$\underline{R}_3 \underline{S}_2$
$C_6$	$\underline{I}$	$\underline{S}_1$	$\underline{S}_1$	$\underline{D}_3$	$\underline{D}_3 \underline{S}_1$	$\underline{D}_3 \underline{S}_2$
$\Gamma_1$	1	1	1	1	1	1
$\Gamma_2$	1	$\omega$	$\omega^2$	1	$\omega$	$\omega^2$
$\Gamma_3$	1	$\omega^2$	$\omega$	1	$\omega^2$	$\omega$
$\Gamma_4$	1	1	1	-1	-1	-1
$\Gamma_5$	1	$\omega$	$\omega^2$	-1	$-\omega$	$-\omega^2$
$\Gamma_6$	1	$\omega^2$	$\omega$	-1	$-\omega^2$	$-\omega$

Table 3.34 Trigonal-dipyramidal class,  $C_{3h}$ 

I.R.	Basic Quantities		$Z_v$
$\Gamma_1$	$T_{11}+T_{22}, T_{33}$	$G_{11}+G_{22}, G_{33}$	$1+3x^3+2x^4+2x^5+3x^6+x^9$
$\Gamma_2$	$T_{11}-T_{22}+2iT_{12}$ $P_1-iP_2$	$G_{11}-G_{22}+2iG_{12}$	$x+2x^2+x^3+2x^4+2x^5+x^6+2x^7+x^8$
$\Gamma_3$	$T_{11}-T_{22}-2iT_{12}$ $P_1+iP_2$	$G_{11}-G_{22}-2iG_{12}$	$x+2x^2+x^3+2x^4+2x^5+x^6+2x^7+x^8$
$\Gamma_4$	$P_3$		$2x^2+4x^3+4x^6+2x^7$
$\Gamma_5$	$T_{31}-iT_{23}$	$G_{31}-iG_{23}$	$x+x^2+x^3+3x^4+3x^5+x^6+x^7+x^8$
$\Gamma_6$	$T_{31}+iT_{23}$	$G_{31}+iG_{23}$	$x+x^2+x^3+3x^4+3x^5+x^6+x^7+x^8$

I.R.	Canonical Expressions
$\Gamma_1$	$a_0 + \sum_{i=1}^8 a_i L_i + a_9 L_1^2 + a_{10} L_2 L_3 + a_{11} L_1 L_4$
$\Gamma_2$	$\sum_{i=1}^5 b_i J_i + (b_6 L_1 + b_7 L_2 + b_8 L_3) J_1 + (b_9 L_1 + b_{10} L_2) J_2 + b_{11} L_6 J_3 +$ $+ b_{12} L_5 J_4$
$\Gamma_3$	$\sum_{i=1}^5 \bar{b}_i \bar{J}_i + (\bar{b}_6 L_1 + \bar{b}_7 L_2 + \bar{b}_8 L_3) \bar{J}_1 + (\bar{b}_9 L_1 + \bar{b}_{10} L_2) \bar{J}_2 + \bar{b}_{11} L_6 \bar{J}_3 +$ $+ \bar{b}_{12} L_5 \bar{J}_4$
$\Gamma_4$	$\sum_{i=1}^6 c_i R_i + c_7 L_1 R_3 + c_8 L_1 R_4 + c_9 L_1 R_5 + c_{10} L_1 R_6 + c_{11} L_2 R_1 +$ $+ c_{12} L_2 R_2$
$\Gamma_5$	$\sum_{i=1}^5 d_i N_i + (d_6 L_1 + d_7 L_2 + d_8 L_3 + d_9 L_5) N_1 + d_{10} L_1 N_2 + d_{11} L_2 N_3 +$ $+ d_{12} L_1 N_4$
$\Gamma_6$	$\sum_{i=1}^5 \bar{d}_i \bar{N}_i + (\bar{d}_6 L_1 + \bar{d}_7 L_2 + \bar{d}_8 L_3 + \bar{d}_9 L_5) \bar{N}_1 + \bar{d}_{10} L_1 \bar{N}_2 + \bar{d}_{11} L_2 \bar{N}_3 +$ $+ \bar{d}_{12} L_1 \bar{N}_4$

Table 3.35 Hexagonal-pyramidal class,  $C_6$

I.R.	Basic Quantities		$Z_v$
$\Gamma_1$	$T_{11}+T_{22}, T_{33}$ $P_3$	$G_{11}+G_{22}, G_{33}$	$1+3x^3+2x^4+2x^5+3x^6+x^9$
$\Gamma_2$	$T_{11}-T_{22}+2iT_{12}$	$G_{11}-G_{22}+2iG_{12}$	$x+2x^2+x^3+2x^4+2x^5+x^6+2x^7+x^8$
$\Gamma_3$	$T_{11}-T_{22}-2iT_{12}$	$G_{11}-G_{22}-2iG_{12}$	$x+2x^2+x^3+2x^4+2x^5+x^6+2x^7+x^8$
$\Gamma_4$			$2x^2+4x^3+4x^6+2x^7$
$\Gamma_5$	$T_{31}-iT_{23}$ $P_1-iP_2$	$G_{31}-iG_{23}$	$x+x^2+x^3+3x^4+3x^5+x^6+x^7+x^8$
$\Gamma_6$	$T_{31}+iT_{23}$ $P_1+iP_2$	$G_{31}+iG_{23}$	$x+x^2+x^3+3x^4+3x^5+x^6+x^7+x^8$
I.R.	Canonical Expressions		
$\Gamma_1$	$a_0 + \sum_{i=1}^8 a_i L_i + a_9 L_1^2 + a_{10} L_2 L_3 + a_{11} L_1 L_4$		
$\Gamma_2$	$\sum_{i=1}^5 b_i J_i + (b_6 L_1 + b_7 L_2 + b_8 L_3) J_1 + (b_9 L_1 + b_{10} L_2) J_2 + b_{11} L_6 J_3 +$ $+ b_{12} L_5 J_4$		
$\Gamma_3$	$\sum_{i=1}^5 \bar{b}_i \bar{J}_i + (\bar{b}_6 L_1 + \bar{b}_7 L_2 + \bar{b}_8 L_3) \bar{J}_1 + (\bar{b}_9 L_1 + \bar{b}_{10} L_2) \bar{J}_2 + \bar{b}_{11} L_6 \bar{J}_3 +$ $+ \bar{b}_{12} L_5 \bar{J}_4$		
$\Gamma_4$	$\sum_{i=1}^6 c_i R_i + c_7 L_1 R_3 + c_8 L_1 R_4 + c_9 L_1 R_5 + c_{10} L_1 R_6 + c_{11} L_2 R_1 +$ $+ c_{12} L_2 R_2$		
$\Gamma_5$	$\sum_{i=1}^5 d_i N_i + (d_6 L_1 + d_7 L_2 + d_8 L_3 + d_9 L_5) N_1 + d_{10} L_1 N_2 + d_{11} L_2 N_3 +$ $+ d_{12} L_1 N_4$		
$\Gamma_6$	$\sum_{i=1}^5 \bar{d}_i \bar{N}_i + (\bar{d}_6 L_1 + \bar{d}_7 L_2 + \bar{d}_8 L_3 + \bar{d}_9 L_5) \bar{N}_1 + \bar{d}_{10} L_1 \bar{N}_2 + \bar{d}_{11} L_2 \bar{N}_3 +$ $+ \bar{d}_{12} L_1 \bar{N}_4$		

We employ below the notation

$$g = G_{31} - iG_{23} \quad , \quad \bar{g} = G_{31} + iG_{23} \quad , \quad G = G_{11} - G_{22} + 2iG_{12} \quad , \\ \bar{G} = G_{11} - G_{22} - 2iG_{12} \quad .$$

Integrity Basis:  $C_{3h}$  ,  $C_6$

$$K_1, \dots, K_6 = G_{11} + G_{22} \quad , \quad G\bar{G} \quad , \quad G^3 + \bar{G}^3 \quad , \quad G_{33} \quad , \quad g\bar{g} \quad , \quad g^6 + \bar{g}^6 \\ L_1 = g^2 G + \bar{g}^2 \bar{G} \quad , \quad L_2 = G\bar{g}^4 + \bar{G}g^4 \quad , \quad L_3 = G^2 \bar{g}^2 + \bar{G}^2 g^2 \quad , \quad L_4 = g^2 G - \bar{g}^2 \bar{G} \quad , \\ L_5 = G^3 - \bar{G}^3 \quad , \quad L_6 = g^6 - \bar{g}^6 \quad , \quad L_7 = G^2 \bar{g}^2 - \bar{G}^2 g^2 \quad , \quad L_8 = G\bar{g}^4 - \bar{G}g^4 \quad .$$

Quantities of type  $\Gamma_2$  appearing in Tables 3.34 and 3.35

$$J_1, \dots, J_5 = G \quad , \quad \bar{g}^2 \quad , \quad \bar{G}^2 \quad , \quad g^4 \quad , \quad \bar{G}g^2$$

Quantities of type  $\Gamma_3$  appearing in Tables 3.34 and 3.35

$$\bar{J}_1, \dots, \bar{J}_5 = \bar{G} \quad , \quad g^2 \quad , \quad G^2 \quad , \quad \bar{g}^4 \quad , \quad G\bar{g}^2$$

Quantities of type  $\Gamma_4$  appearing in Tables 3.34 and 3.35

$$R_1, \dots, R_6 = G\bar{g} + \bar{G}g \quad , \quad G\bar{g} - \bar{G}g \quad , \quad g^3 + \bar{g}^3 \quad , \quad g^3 - \bar{g}^3 \quad , \quad G^2 g + \bar{G}^2 \bar{g} \quad , \quad G^2 g - \bar{G}^2 \bar{g}$$

Quantities of type  $\Gamma_5$  appearing in Tables 3.34 and 3.35

$$N_1, \dots, N_5 = g \quad , \quad \bar{G}g \quad , \quad R_2 G \quad , \quad R_4 G \quad , \quad R_3 \bar{g}^2$$

Quantities of type  $\Gamma_6$  appearing in Tables 3.34 and 3.35

$$\bar{N}_1, \dots, \bar{N}_5 = \bar{g} \quad , \quad Gg \quad , \quad R_2 \bar{G} \quad , \quad R_4 \bar{G} \quad , \quad R_3 g^2$$

Generating Function:  $C_{3h}$  ,  $C_6$

$$GF(\Gamma_v) = \frac{Z_v}{(1-x)^2 (1-x^2)^2 (1-x^3) (1-x^6)}$$

- 3.3.10 Ditrigonal-dipyramidal class,  $D_{3h}, (\underline{I}, \underline{R}_1, \underline{R}_3, \underline{D}_2) \cdot (\underline{I}, \underline{S}_1, \underline{S}_2)$   
Hexagonal-scalenohedral class,  $D_{3d}, (\underline{I}, \underline{C}, \underline{R}_1, \underline{D}_1) \cdot (\underline{I}, \underline{S}_1, \underline{S}_2)$   
Hexagonal-trapezohedral class,  $D_6, (\underline{I}, \underline{D}_1, \underline{D}_2, \underline{D}_3) \cdot (\underline{I}, \underline{S}_1, \underline{S}_2)$   
Dihexagonal-pyramidal class,  $C_{6v}, (\underline{I}, \underline{R}_1, \underline{R}_2, \underline{D}_3) \cdot (\underline{I}, \underline{S}_1, \underline{S}_2)$

Table 3.36 Irreducible Representations:  $D_{3h}, D_{3d}, D_6, C_{6v}$

	$\underline{I}$	$\underline{S}_1$	$\underline{S}_2$	$\underline{R}_3$	$\underline{R}_3 \underline{S}_1$	$\underline{R}_3 \underline{S}_2$	$\underline{R}_1$	$\underline{R}_1 \underline{S}_1$	$\underline{R}_1 \underline{S}_2$	$\underline{D}_2$	$\underline{D}_2 \underline{S}_1$	$\underline{D}_2 \underline{S}_2$
$D_{3h}$	$\underline{I}$	$\underline{S}_1$	$\underline{S}_2$	$\underline{R}_3$	$\underline{R}_3 \underline{S}_1$	$\underline{R}_3 \underline{S}_2$	$\underline{R}_1$	$\underline{R}_1 \underline{S}_1$	$\underline{R}_1 \underline{S}_2$	$\underline{D}_2$	$\underline{D}_2 \underline{S}_1$	$\underline{D}_2 \underline{S}_2$
	$\underline{I}$	$\underline{S}_1$	$\underline{S}_2$	$\underline{C}$	$\underline{C} \underline{S}_1$	$\underline{C} \underline{S}_2$	$\underline{D}_1$	$\underline{D}_1 \underline{S}_1$	$\underline{D}_1 \underline{S}_2$	$\underline{R}_1$	$\underline{R}_1 \underline{S}_1$	$\underline{R}_1 \underline{S}_2$
$D_{3d}$	$\underline{I}$	$\underline{S}_1$	$\underline{S}_2$	$\underline{C}$	$\underline{C} \underline{S}_1$	$\underline{C} \underline{S}_2$	$\underline{D}_1$	$\underline{D}_1 \underline{S}_1$	$\underline{D}_1 \underline{S}_2$	$\underline{R}_1$	$\underline{R}_1 \underline{S}_1$	$\underline{R}_1 \underline{S}_2$
	$\underline{I}$	$\underline{S}_1$	$\underline{S}_2$	$\underline{D}_3$	$\underline{D}_3 \underline{S}_1$	$\underline{D}_3 \underline{S}_2$	$\underline{D}_1$	$\underline{D}_1 \underline{S}_1$	$\underline{D}_1 \underline{S}_2$	$\underline{D}_2$	$\underline{D}_2 \underline{S}_1$	$\underline{D}_2 \underline{S}_2$
$D_6$	$\underline{I}$	$\underline{S}_1$	$\underline{S}_2$	$\underline{D}_3$	$\underline{D}_3 \underline{S}_1$	$\underline{D}_3 \underline{S}_2$	$\underline{D}_1$	$\underline{D}_1 \underline{S}_1$	$\underline{D}_1 \underline{S}_2$	$\underline{D}_2$	$\underline{D}_2 \underline{S}_1$	$\underline{D}_2 \underline{S}_2$
	$\underline{I}$	$\underline{S}_1$	$\underline{S}_2$	$\underline{D}_3$	$\underline{D}_3 \underline{S}_1$	$\underline{D}_3 \underline{S}_2$	$\underline{R}_2$	$\underline{R}_2 \underline{S}_1$	$\underline{R}_2 \underline{S}_2$	$\underline{R}_1$	$\underline{R}_1 \underline{S}_1$	$\underline{R}_1 \underline{S}_2$
$C_{6v}$	$\underline{I}$	$\underline{S}_1$	$\underline{S}_2$	$\underline{D}_3$	$\underline{D}_3 \underline{S}_1$	$\underline{D}_3 \underline{S}_2$	$\underline{R}_2$	$\underline{R}_2 \underline{S}_1$	$\underline{R}_2 \underline{S}_2$	$\underline{R}_1$	$\underline{R}_1 \underline{S}_1$	$\underline{R}_1 \underline{S}_2$
$\Gamma_1$	1	1	1	1	1	1	1	1	1	1	1	1
$\Gamma_2$	1	1	1	1	1	1	-1	-1	-1	-1	-1	-1
$\Gamma_3$	1	1	1	-1	-1	-1	1	1	1	-1	-1	-1
$\Gamma_4$	1	1	1	-1	-1	-1	-1	-1	-1	1	1	1
$\Gamma_5$	E	A	B	-E	-A	-B	F	G	H	-F	-G	-H
$\Gamma_6$	E	A	B	E	A	B	-F	-G	-H	-F	-G	-H

The matrices  $\underline{E}, \dots, \underline{H}$  appearing in Table 3.36 are defined in section 3.3.8.

Table 3.37 Ditrigonal-dipyramidal class,  $D_{3h}$

I.R.	Basic Quantities		$Z_v$
$\Gamma_1$	$T_{11}+T_{22}, T_{33}$	$G_{11}+G_{22}, G_{33}$	$1+x^3+x^4+x^5+x^6+x^9$
$\Gamma_3$	$P_3$		$x^2+2x^3+2x^6+x^7$
$\Gamma_5$	$(T_{23}, -T_{31})^T$	$(G_{23}, -G_{31})^T$	$x+x^2+x^3+3x^4+3x^5+x^6+x^7+x^8$
$\Gamma_6$	$(2T_{12}, T_{11}-T_{22})^T$ $(P_1, P_2)^T$	$(2G_{12}, G_{11}-G_{22})^T$	$x+2x^2+x^3+2x^4+2x^5+x^6+$ $+2x^7+x^8$

I.R.	Canonical Expressions
$\Gamma_1$	$a_0 + a_1 L_1 + a_2 L_2 + a_3 L_3 + a_4 L_1^2 + a_5 L_2 L_3$
$\Gamma_3$	$b_1 I_1 + b_2 I_2 + b_3 I_3 + b_4 L_1 I_2 + b_5 L_1 I_3 + b_6 L_2 I_1$
$\Gamma_5$	$\sum_{i=1}^6 c_i J_i + (c_7 L_1 + c_8 L_2 + c_9 L_3) J_1 + c_{10} L_1 J_2 + c_{11} L_2 J_3 + c_{12} L_1 J_5$
$\Gamma_6$	$\sum_{i=1}^5 d_i R_i + (d_6 L_1 + d_7 L_2) R_1 + (d_8 L_1 + d_9 L_2) R_2 + (d_{10} L_1 + d_{11} L_2) R_3 +$ $+ d_{12} L_3 R_4$

For the class  $D_{3h}$ , we employ the notation

$$g = G_{23} - iG_{31}, \quad \bar{g} = G_{23} + iG_{31}, \quad G = 2G_{12} + i(G_{11} - G_{22}),$$

$$\bar{G} = 2G_{12} - i(G_{11} - G_{22}).$$

Integrity Basis:  $D_{3h}$

$$K_1, \dots, K_6 = G_{11} + G_{22}, G\bar{G}, G^3 - \bar{G}^3, G_{33}, g\bar{g}, g^6 + \bar{g}^6$$

$$L_1, \dots, L_3 = g^2 G - \bar{g}^2 \bar{G}, g^4 \bar{G} - \bar{g}^4 G, g^2 \bar{G}^2 + \bar{g}^2 G^2$$



Quantities of type  $\Gamma_3 : D_{3h}$

$$I_1, \dots, I_3 = G\bar{g} - \bar{G}g, g^3 + \bar{g}^3, G^2g + \bar{G}^2\bar{g}$$

Quantities of type  $\Gamma_5 : D_{3h}$

$$\tilde{J}_1 = \begin{vmatrix} G_{23} \\ -G_{31} \end{vmatrix}, \tilde{J}_2 = \begin{vmatrix} (G_{11} - G_{22})G_{23} - 2G_{12}G_{31} \\ (G_{11} - G_{22})G_{31} + 2G_{12}G_{23} \end{vmatrix}, \tilde{J}_3 = (G\bar{g} + \bar{G}g) \begin{vmatrix} 2G_{12} \\ G_{11} - G_{22} \end{vmatrix},$$

$$\tilde{J}_4 = (G^3 + \bar{G}^3) \begin{vmatrix} G_{31} \\ G_{23} \end{vmatrix}, \tilde{J}_5 = (g^3 + \bar{g}^3) \begin{vmatrix} 2G_{12} \\ G_{11} - G_{22} \end{vmatrix}, \tilde{J}_6 = (g^3 + \bar{g}^3) \begin{vmatrix} G_{23}^2 - G_{31}^2 \\ 2G_{23}G_{31} \end{vmatrix}$$

Quantities of type  $\Gamma_6 : D_{3h}$

$$\tilde{R}_1 = \begin{vmatrix} 2G_{12} \\ G_{11} - G_{22} \end{vmatrix}, \tilde{R}_2 = \begin{vmatrix} 2G_{23}G_{31} \\ G_{31}^2 - G_{23}^2 \end{vmatrix}, \tilde{R}_3 = \begin{vmatrix} -4(G_{11} - G_{22})G_{12} \\ (G_{11} - G_{22})^2 - 4G_{12}^2 \end{vmatrix},$$

$$\tilde{R}_4 = \begin{vmatrix} 4G_{23}G_{31}(G_{31}^2 - G_{23}^2) \\ 4G_{23}^2G_{31}^2 - (G_{31}^2 - G_{23}^2)^2 \end{vmatrix}, \tilde{R}_5 = \begin{vmatrix} 2(G_{11} - G_{22})G_{23}G_{31} + 2G_{12}(G_{31}^2 - G_{23}^2) \\ -(G_{11} - G_{22})(G_{31}^2 - G_{23}^2) + 4G_{12}G_{23}G_{31} \end{vmatrix}$$

Generating Function:  $D_{3h}$

$$GF(\Gamma_v) = \frac{Z_v}{(1-x)^2(1-x^2)^2(1-x^3)(1-x^6)}$$

Table 3.38 Hexagonal-scalenohedral class,  $D_{3d}$

I.R.	Basic Quantities		$Z_V$
$\Gamma_1$	$T_{11}+T_{22}, T_{33}$	$G_{11}+G_{22}, G_{33}$	$1+x^2+2x^3+x^4+x^6$
$\Gamma_4$	$P_3$		0
$\Gamma_5$	$(P_1, P_2)^T$		0
$\Gamma_6$	$(T_{31}, T_{23})^T$ $(2T_{12}, T_{11}-T_{22})^T$	$(G_{31}, G_{23})^T$ $(2G_{12}, G_{11}-G_{22})^T$	$2x+3x^2+2x^3+3x^4+2x^5$

I.R.	Canonical Expressions
$\Gamma_1$	$a_0 + a_1 L_1 + a_2 L_2 + a_3 L_3 + a_4 L_1^2 + a_5 L_2 L_3$
$\Gamma_4$	None
$\Gamma_5$	None
$\Gamma_6$	$\sum_{i=1}^5 b_i J_i + (b_6 L_1 + b_7 L_2) J_1 + (b_8 L_1 + b_9 L_2) J_2 + (b_{10} L_1 + b_{11} L_2) J_3 +$ $+ b_{12} L_3 J_4$

For the class  $D_{3d}$ , we employ the notation

$$g = G_{31} + iG_{23}, \quad \bar{g} = G_{31} - iG_{23}, \quad G = 2G_{12} + i(G_{11} - G_{22}),$$

$$\bar{G} = 2G_{12} - i(G_{11} - G_{22}).$$

Integrity Basis:  $D_{3d}$

$$K_1, \dots, K_6 = G_{11} + G_{22}, G\bar{G}, G^3 - \bar{G}^3, G_{33}, g\bar{g}, g^3 - \bar{g}^3$$

$$L_1, \dots, L_3 = g\bar{G} + \bar{g}G, Gg^2 - \bar{G}\bar{g}^2, G^2g - \bar{G}^2\bar{g}$$

Quantities of type  $\Gamma_6 : D_{3d}$

$$J_1 = \left\| \begin{array}{c} 2G_{12} \\ G_{11}-G_{22} \end{array} \right\|, \quad J_2 = \left\| \begin{array}{c} G_{31} \\ G_{23} \end{array} \right\|, \quad J_3 = \left\| \begin{array}{c} -4(G_{11}-G_{22})G_{12} \\ (G_{11}-G_{22})^2-4G_{12}^2 \end{array} \right\|$$

$$J_4 = \left\| \begin{array}{c} 2G_{23}G_{31} \\ G_{31}^2-G_{23}^2 \end{array} \right\|, \quad J_5 = \left\| \begin{array}{c} (G_{11}-G_{22})G_{31}+2G_{12}G_{23} \\ -(G_{11}-G_{22})G_{23}+2G_{12}G_{31} \end{array} \right\|$$

Generating Function:  $D_{3d}$

$$GF(\Gamma_v) = \frac{Z_v}{(1-x)^2(1-x^2)^2(1-x^3)^2}$$

Table 3.39 Hexagonal-trapezohedral class,  $D_6$

I.R.	Basic Quantities		$Z_v$
$\Gamma_1$	$T_{11}+T_{22}, T_{33}$	$G_{11}+G_{22}, G_{33}$	$1+x^3+x^4+x^5+x^6+x^9$
$\Gamma_2$	$P_3$		$2x^3+x^4+x^5+2x^6$
$\Gamma_5$	$(T_{23}, -T_{31})^T$ $(P_1, P_2)^T$	$(G_{23}, -G_{31})^T$	$x+x^2+x^3+3x^4+3x^5+x^6+$ $+x^7+x^8$
$\Gamma_6$	$(2T_{12}, T_{11}-T_{22})^T$	$(2G_{12}, G_{11}-G_{22})^T$	$x+2x^2+x^3+2x^4+2x^5+x^6+$ $+2x^7+x^8$

I.R.	Canonical Expressions
$\Gamma_1$	$a_0 + a_1 L_1 + a_2 L_2 + a_3 L_3 + a_4 L_1^2 + a_5 L_2 L_3$
$\Gamma_2$	$\sum_{i=1}^5 b_i M_i + b_6 L_1 M_1$
$\Gamma_5$	$\sum_{i=1}^6 c_i J_i + (c_7 L_1 + c_8 L_2 + c_9 L_3) J_1 + c_{10} L_1 J_2 + c_{11} L_2 J_3 + c_{12} L_1 J_5$
$\Gamma_6$	$\sum_{i=1}^5 d_i R_i + (d_6 L_1 + d_7 L_2) R_1 + (d_8 L_1 + d_9 L_2) R_2$ $+ (d_{10} L_1 + d_{11} L_2) R_3 + d_{12} L_3 R_4$

For the class  $D_6$ , we employ the notation

$$g = G_{23} - iG_{31} \quad , \quad \bar{g} = G_{23} + iG_{31} \quad , \quad G = 2G_{12} + i(G_{11} - G_{22}) \quad ,$$

$$\bar{G} = 2G_{12} - i(G_{11} - G_{22}) \quad .$$

Integrity Basis:  $D_6$

$$K_1, \dots, K_6 = G_{11} + G_{22} \quad , \quad G\bar{G} \quad , \quad G^3 - \bar{G}^3 \quad , \quad G_{33} \quad , \quad g\bar{g} \quad , \quad g^6 + \bar{g}^6$$

$$L_1, \dots, L_3 = g^2 G - \bar{g}^2 \bar{G} \quad , \quad g^4 \bar{G} - \bar{g}^4 G \quad , \quad g^2 \bar{G}^2 + \bar{g}^2 G^2$$

Quantities of type  $\Gamma_2: D_6$

$$M_1, \dots, M_5 = Gg^2 + \bar{G}\bar{g}^2, \quad G^3 + \bar{G}^3, \quad g^6 - \bar{g}^6, \quad G^2\bar{g}^2 - \bar{G}^2g^2, \quad G\bar{g}^4 + \bar{G}g^4$$

Quantities of type  $\Gamma_5: D_6$

$$\underline{J}_1 = \begin{vmatrix} G_{23} \\ -G_{31} \end{vmatrix}, \quad \underline{J}_2 = \begin{vmatrix} (G_{11} - G_{22})G_{23} - 2G_{12}G_{31} \\ (G_{11} - G_{22})G_{31} + 2G_{12}G_{23} \end{vmatrix}, \quad \underline{J}_3 = (G\bar{g} + \bar{G}g) \begin{vmatrix} 2G_{12} \\ G_{11} - G_{22} \end{vmatrix}.$$

$$\underline{J}_4 = (G^3 + \bar{G}^3) \begin{vmatrix} G_{31} \\ G_{23} \end{vmatrix}, \quad \underline{J}_5 = (g^3 - \bar{g}^3) \begin{vmatrix} 2G_{12} \\ G_{11} - G_{22} \end{vmatrix}, \quad \underline{J}_6 = (g^3 + \bar{g}^3) \begin{vmatrix} G_{23}^2 - G_{31}^2 \\ 2G_{23}G_{31} \end{vmatrix}$$

Quantities of type  $\Gamma_6: D_6$

$$\underline{R}_1 = \begin{vmatrix} 2G_{12} \\ G_{11} - G_{22} \end{vmatrix}, \quad \underline{R}_2 = \begin{vmatrix} 2G_{23}G_{31} \\ G_{31}^2 - G_{23}^2 \end{vmatrix}, \quad \underline{R}_3 = \begin{vmatrix} -4(G_{11} - G_{22})G_{12} \\ (G_{11} - G_{22})^2 - 4G_{12}^2 \end{vmatrix},$$

$$\underline{R}_4 = \begin{vmatrix} 4G_{23}G_{31}(G_{31}^2 - G_{23}^2) \\ 4G_{23}^2G_{31}^2 - (G_{31}^2 - G_{23}^2)^2 \end{vmatrix}, \quad \underline{R}_5 = \begin{vmatrix} 2(G_{11} - G_{22})G_{23}G_{31} + 2G_{12}(G_{31}^2 - G_{23}^2) \\ -(G_{11} - G_{22})(G_{31}^2 - G_{23}^2) + 4G_{12}G_{23}G_{31} \end{vmatrix}$$

Generating Function:  $D_6$

$$GF(\Gamma_v) = \frac{Z_v}{(1-x)^2(1-x^2)^2(1-x^3)(1-x^6)}$$

Table 3.40 Dihexagonal-pyramidal class,  $C_{6v}$

I.R.	Basic Quantities		$Z_v$
$\Gamma_1$	$T_{11}+T_{22}, T_{33}$ $P_3$		$1+x^3+x^4+x^5+x^6+x^9$ $x+x^2+x^3+3x^4+3x^5+x^6+$ $+x^7+x^8$
$\Gamma_5$	$(T_{31}, T_{23})^T$ $(P_1, P_2)^T$	$(G_{31}, G_{23})^T$	
$\Gamma_6$	$(2T_{12}, T_{11}-T_{22})^T$	$(2G_{12}, G_{11}-G_{22})^T$	$x+2x^2+x^3+2x^4+2x^5+x^6+$ $+2x^7+x^8$

I.R.	Canonical Expressions
$\Gamma_1$	$a_0 + a_1 L_1 + a_2 L_2 + a_3 L_3 + a_4 L_1^2 + a_5 L_2 L_3$
$\Gamma_5$	$\sum_{i=1}^6 b_i J_{\sim i} + (b_7 L_1 + b_8 L_2 + b_9 L_3) J_{\sim 1} + b_{10} L_1 J_{\sim 2} + b_{11} L_2 J_{\sim 3} + b_{12} L_1 J_{\sim 5}$
$\Gamma_6$	$\sum_{i=1}^5 c_i R_{\sim i} + (c_6 L_1 + c_7 L_2) R_{\sim 1} + (c_8 L_1 + c_9 L_2) R_{\sim 2} + (c_{10} L_1 + c_{11} L_2) R_{\sim 3} + c_{12} L_3 R_{\sim 4}$

For the class  $C_{6v}$ , we employ the notation

$$g = G_{31} + iG_{23} \quad , \quad \bar{g} = G_{31} - iG_{23} \quad , \quad G = 2G_{12} + i(G_{11} - G_{22}) \quad ,$$

$$\bar{G} = 2G_{12} - i(G_{11} - G_{22}) \quad .$$

Integrity Basis:  $C_{6v}$

$$K_1, \dots, K_5 = G_{11} + G_{22} \quad , \quad G\bar{G} \quad , \quad G^3 - \bar{G}^3 \quad , \quad G_{33} \quad , \quad g\bar{g} \quad , \quad g^6 + \bar{g}^6$$

$$L_1 = g^2 G - \bar{g}^2 \bar{G} \quad , \quad L_2 = g^4 \bar{G} - \bar{g}^4 G \quad , \quad L_3 = g^2 \bar{G}^2 + \bar{g}^2 G^2$$

Quantities of type  $\Gamma_5: C_{6v}$

$$\begin{aligned} \underline{J}_1 &= \begin{vmatrix} G_{31} \\ G_{23} \end{vmatrix}, \underline{J}_2 = \begin{vmatrix} (G_{11}-G_{22})G_{31}+2G_{12}G_{23} \\ -(G_{11}-G_{22})G_{23}+2G_{12}G_{31} \end{vmatrix}, \underline{J}_3 = (G\bar{g}+\bar{G}g) \begin{vmatrix} 2G_{12} \\ G_{11}-G_{22} \end{vmatrix}, \\ \underline{J}_4 &= (G^3+\bar{G}^3) \begin{vmatrix} G_{23} \\ -G_{31} \end{vmatrix}, \underline{J}_5 = (g^3-\bar{g}^3) \begin{vmatrix} 2G_{12} \\ G_{11}-G_{22} \end{vmatrix}, \underline{J}_6 = (g^3+\bar{g}^3) \begin{vmatrix} G_{31}^2-G_{23}^2 \\ -2G_{23}G_{31} \end{vmatrix} \end{aligned}$$

Quantities of type  $\Gamma_6: C_{6v}$

$$\begin{aligned} \underline{R}_1 &= \begin{vmatrix} 2G_{12} \\ G_{11}-G_{22} \end{vmatrix}, \underline{R}_2 = \begin{vmatrix} 2G_{23}G_{31} \\ G_{31}^2-G_{23}^2 \end{vmatrix}, \underline{R}_3 = \begin{vmatrix} -4(G_{11}-G_{22})G_{12} \\ (G_{11}-G_{22})-4G_{12}^2 \end{vmatrix}, \\ \underline{R}_4 &= \begin{vmatrix} 4G_{23}G_{31}(G_{31}^2-G_{23}^2) \\ 4G_{23}^2G_{31}^2-(G_{31}^2-G_{23}^2)^2 \end{vmatrix}, \underline{R}_5 = \begin{vmatrix} 2(G_{11}-G_{22})G_{23}G_{31}+2G_{12}(G_{31}^2-G_{23}^2) \\ -(G_{11}-G_{22})(G_{31}^2-G_{23}^2)+4G_{12}G_{23}G_{31} \end{vmatrix} \end{aligned}$$

Generating Function:  $C_{6v}$

$$GF(\Gamma_v) = \frac{Z_v}{(1-x)^2(1-x^2)^2(1-x^3)(1-x^6)}$$

### 3.3.11 Dihexagonal-dipyramidal class,

$$D_{6h} = (I, C, R_1, R_2, R_3, D_1, D_2, D_3) \cdot (I, S_1, S_2)$$

Table 3.41 Irreducible Representations:  $D_{6h}$

$D_{6h}$	I	$S_1$	$S_2$	$D_1$	$D_1S_1$	$D_1S_2$	$D_2$	$D_2S_1$	$D_2S_2$	$D_3$	$D_3S_1$	$D_3S_2$
$\Gamma_1$	1	1	1	1	1	1	1	1	1	1	1	1
$\Gamma_2$	1	1	1	-1	-1	-1	-1	-1	-1	1	1	1
$\Gamma_3$	1	1	1	1	1	1	-1	-1	-1	-1	-1	-1
$\Gamma_4$	1	1	1	-1	-1	-1	1	1	1	-1	-1	-1
$\Gamma_5$	E	A	B	F	G	H	-F	-G	-H	-E	-A	-B
$\Gamma_6$	E	A	B	-F	-G	-H	-F	-G	-H	E	A	B
$\Gamma'_1$	1	1	1	1	1	1	1	1	1	1	1	1
$\Gamma'_2$	1	1	1	-1	-1	-1	-1	-1	-1	1	1	1
$\Gamma'_3$	1	1	1	1	1	1	-1	-1	-1	-1	-1	-1
$\Gamma'_4$	1	1	1	-1	-1	-1	1	1	1	-1	-1	-1
$\Gamma'_5$	E	A	B	F	G	H	-F	-G	-H	-E	-A	-B
$\Gamma'_6$	E	A	B	-F	-G	-H	-F	-G	-H	E	A	B

(continued)



Table 3.41 Irreducible Representations:  $D_{6h}$  (continued)

$D_{6h}$	C	$CS_1$	$CS_2$	$R_1$	$R_1S_1$	$R_1S_2$	$R_2$	$R_2S_1$	$R_2S_2$	$R_3$	$R_3S_1$	$R_3S_2$
$\Gamma_1$	1	1	1	1	1	1	1	1	1	1	1	1
$\Gamma_2$	1	1	1	-1	-1	-1	-1	-1	-1	1	1	1
$\Gamma_3$	1	1	1	1	1	1	1	-1	-1	-1	-1	-1
$\Gamma_4$	1	1	1	-1	-1	-1	1	1	1	-1	-1	-1
$\Gamma_5$	E	A	B	F	G	H	-F	-G	-H	-E	-A	-B
$\Gamma_6$	E	A	B	-F	-G	-H	-F	-G	-H	E	A	B
$\Gamma'_1$	-1	-1	-1	-1	-1	-1	-1	-1	-1	-1	-1	-1
$\Gamma'_2$	-1	-1	-1	1	1	1	1	1	1	-1	-1	-1
$\Gamma'_3$	-1	-1	-1	-1	-1	-1	1	1	1	1	1	1
$\Gamma'_4$	-1	-A	-B	1	1	1	-1	-1	-1	1	1	1
$\Gamma'_5$	-E	-A	-B	-F	-G	-H	F	G	H	E	A	B
$\Gamma'_6$	-E		-B	F	G	H	F	G	H	-E	-A	-B

The matrices  $\underline{E}, \dots, \underline{H}$  appearing in Table 3.41 are defined in section 3.3.8.

Table 3.42 Dihexagonal-dipyramidal class,  $D_{6h}$

I.R.	Basic Quantities		$Z_v$
$\Gamma_1$	$T_{11}+T_{22}, T_{33}$	$G_{11}+G_{22}, G_{33}$	$1+x^3+x^4+x^5+x^6+x^9$
$\Gamma_5$	$(T_{23}, -T_{31})^T$	$(G_{23}, -G_{31})^T$	$x + x^2+x^3+3x^4+3x^5+x^6+x^7+x^8$
$\Gamma_6$	$(2T_{12}, T_{11}-T_{22})^T$	$(2G_{12}, G_{11}-G_{22})^T$	$x+2x^2+x^3+2x^4+2x^5+x^6+2x^7+x^8$
$\Gamma'_2$	$P_3$		0
$\Gamma'_5$	$(P_1, P_2)^T$		0

I.R.	Canonical Expressions
$\Gamma_1$	$a_0 + a_1 L_1 + a_2 L_2 + a_3 L_3 + a_4 L_1^2 + a_5 L_2 L_3$
$\Gamma_5$	$\sum_{i=1}^6 b_i J_i + (b_7 L_1 + b_8 L_2 + b_9 L_3) J_1 + b_{10} L_1 J_2 + b_{11} L_2 J_3 + b_{12} L_1 J_5$
$\Gamma_6$	$\sum_{i=1}^6 c_i R_i + (c_6 L_1 + c_7 L_2) R_1 + (c_8 L_1 + c_9 L_2) R_2 + (c_{10} L_1 + c_{11} L_2) R_3$ $+ c_{12} L_3 R_4$
$\Gamma'_2$	None
$\Gamma'_5$	None

For the class  $D_{6h}$ , we employ the notation

$$g = G_{23} - iG_{31}, \quad \bar{g} = G_{23} + iG_{31}, \quad G = 2G_{12} + i(G_{11} - G_{22}),$$

$$\bar{G} = 2G_{12} - i(G_{11} - G_{22}).$$

Integrity Basis:  $D_{6h}$

$$K_1, \dots, K_6 = G_{11} + G_{12}, \quad G\bar{G}, \quad G^3 - \bar{G}^3, \quad G_{33}, \quad g\bar{g}, \quad g^6 + \bar{g}^6$$

$$L_1, \dots, L_3 = g^2 G - \bar{g}^2 \bar{G}, \quad g^4 \bar{G} - \bar{g}^4 G, \quad g^2 \bar{G}^2 + \bar{g}^2 G^2$$

Quantities of type  $\Gamma_5 : D_{6h}$

$$J_1 = \begin{vmatrix} G_{23} \\ -G_{31} \end{vmatrix}, \quad J_2 = \begin{vmatrix} (G_{11} - G_{22})G_{23} - 2G_{12}G_{31} \\ (G_{11} - G_{22})G_{31} + 2G_{12}G_{23} \end{vmatrix}, \quad J_3 = (G\bar{g} + \bar{G}g) \begin{vmatrix} 2G_{12} \\ G_{11} - G_{22} \end{vmatrix},$$

$$J_4 = (G^3 + \bar{G}^3) \begin{vmatrix} G_{31} \\ G_{23} \end{vmatrix}, \quad J_5 = (g^3 - \bar{g}^3) \begin{vmatrix} 2G_{12} \\ G_{11} - G_{22} \end{vmatrix}$$

$$J_6 = (g^3 + \bar{g}^3) \begin{vmatrix} G_{23}^2 - G_{31}^2 \\ 2G_{23}G_{31} \end{vmatrix}$$

Quantities of type  $\Gamma_6 : D_{6h}$

$$R_1 = \begin{vmatrix} 2G_{12} \\ G_{11} - G_{22} \end{vmatrix}, \quad R_2 = \begin{vmatrix} 2G_{23}G_{31} \\ G_{31}^2 - G_{23}^2 \end{vmatrix}, \quad R_3 = \begin{vmatrix} -4(G_{11} - G_{22})G_{12} \\ (G_{11} - G_{22})^2 - 4G_{12}^2 \end{vmatrix},$$

$$R_4 = \begin{vmatrix} 4G_{23}G_{31}(G_{31}^2 - G_{23}^2) \\ 4G_{23}^2G_{31}^2 - (G_{31}^2 - G_{23}^2)^2 \end{vmatrix}, \quad R_5 = \begin{vmatrix} 2(G_{11} - G_{22})G_{23}G_{31} + 2G_{12}(G_{31}^2 - G_{23}^2) \\ -(G_{11} - G_{22})(G_{31}^2 - G_{23}^2) + 4G_{12}G_{23}G_{31} \end{vmatrix}$$

Generating Function:  $D_{6h}$

$$GF(\Gamma_v) = \frac{Z_v}{(1-x)^2(1-x^2)^2(1-x^3)(1-x^6)}$$

3.3.12 Tetartoidal class,  $T$ ,  $(\underline{I}, \underline{D}_1, \underline{D}_2, \underline{D}_3) \cdot (\underline{I}, \underline{M}_1, \underline{M}_2)$

Diploidal class,  $T_h$ ,  $(\underline{I}, \underline{C}, \underline{R}_1, \underline{R}_2, \underline{R}_3, \underline{D}_1, \underline{D}_2, \underline{D}_3) \cdot (\underline{I}, \underline{M}_1, \underline{M}_2)$

We note that the general expressions for a second-order tensor-valued function  $T_{ij}(G_{kl})$  of a symmetric second-order tensor which are invariant under the group  $T$  and invariant under the group  $T_h$  are identical. Further, there are no vector-valued functions  $P_i(G_{kl})$  which are invariant under the group  $T_h$ . Hence, we restrict consideration to the group  $T$ . The matrices  $\underline{I}, \underline{D}_1, \dots, \underline{D}_3 \underline{M}_2$  appearing in Table 3.43 are the matrices employed in the description of material symmetry and are defined in section 3.1.

Table 3.43 Irreducible Representations:  $T$

$T$	$\underline{I}$	$\underline{D}_1$	$\underline{D}_2$	$\underline{D}_3$	$\underline{M}_1$	$\underline{D}_1 \underline{M}_1$	$\underline{D}_2 \underline{M}_1$	$\underline{D}_3 \underline{M}_1$	$\underline{M}_2$	$\underline{D}_1 \underline{M}_2$	$\underline{D}_2 \underline{M}_2$	$\underline{D}_3 \underline{M}_2$
$\Gamma_1$	1	1	1	1	1	1	1	1	1	1	1	1
$\Gamma_2$	1	1	1	1	$\omega$	$\omega$	$\omega$	$\omega$	$\omega^2$	$\omega^2$	$\omega^2$	$\omega^2$
$\Gamma_3$	1	1	1	1	$\omega^2$	$\omega^2$	$\omega^2$	$\omega^2$	$\omega$	$\omega$	$\omega$	$\omega$
$\Gamma_4$	$\underline{I}$	$\underline{D}_1$	$\underline{D}_2$	$\underline{D}_3$	$\underline{M}_1$	$\underline{D}_1 \underline{M}_1$	$\underline{D}_2 \underline{M}_1$	$\underline{D}_3 \underline{M}_1$	$\underline{M}_2$	$\underline{D}_1 \underline{M}_2$	$\underline{D}_2 \underline{M}_2$	$\underline{D}_3 \underline{M}_2$

In Table 3.43, the quantities  $\omega$  and  $\omega^2$  are defined by  
 $\omega = -1/2 + i\sqrt{3}/2$ ,  $\omega^2 = -1/2 - i\sqrt{3}/2$ .

Table 3.44 Tetartoidal class,  $T$

I.R.	Basic Quantities		$Z_v$
$\Gamma_1$	$T_{11}+T_{22}+T_{33}$	$G_{11}+G_{22}+G_{33}$	$1+3x^2+2x^4+2x^5+3x^6+x^9$
$\Gamma_2$	$T_{11}+\omega^2 T_{22}+\omega T_{33}$	$G_{11}+\omega^2 G_{22}+\omega G_{33}$	$x+2x^2+x^3+2x^4+2x^5+x^6+2x^7+x^8$
$\Gamma_3$	$T_{11}+\omega T_{22}+\omega^2 T_{33}$	$G_{11}+\omega G_{22}+\omega^2 G_{33}$	$x+2x^2+x^3+2x^4+2x^5+x^6+2x^7+x^8$
$\Gamma_4$	$(T_{23}, T_{31}, T_{12})^T$ $(P_1, P_2, P_3)^T$	$(G_{23}, G_{31}, G_{12})^T$	$x+3x^2+6x^3+8x^4+8x^5+6x^6+3x^7+x^8$

I.R.	Canonical Expressions
$\Gamma_1$	$a_0 + \sum_{i=1}^8 a_i L_i + a_9 L_1^2 + a_{10} L_2 L_3 + a_{11} L_1 L_4$
$\Gamma_2$	
$\Gamma_3$	
$\Gamma_4$	

Integrity Basis:  $T$ ,

$$K_1, \dots, K_6 = \Sigma G_{11}, \Sigma G_{11} G_{22}, G_{11} G_{22} G_{33}, \Sigma G_{23}^2, \Sigma G_{23}^2 G_{31}^2, G_{23} G_{31} G_{12}$$

$$L_1 = \Sigma G_{11} (G_{31}^2 + G_{12}^2), \quad L_2 = \Sigma G_{11} G_{31}^2 G_{12}^2,$$

$$L_3 = \Sigma G_{23}^2 G_{22} G_{33}, \quad L_4 = \Sigma G_{11} (G_{31}^2 - G_{12}^2),$$

$$L_5 = \Sigma G_{11} G_{22} (G_{11} - G_{22}), \quad L_6 = \Sigma G_{23}^2 G_{31}^2 (G_{23}^2 - G_{31}^2),$$

$$L_7 = \Sigma G_{11} G_{22} (G_{31}^2 - G_{23}^2), \quad L_8 = \Sigma G_{23}^2 G_{31}^2 (G_{11} - G_{22})$$

The quantity  $\Sigma G_{i_1 j_1} \dots G_{i_n j_n}$  denotes the sum of the three quantities obtained by permitting the subscripts in the summand cyclically. For example,  $\Sigma G_{11} G_{22} = G_{11} G_{22} + G_{22} G_{33} + G_{33} G_{11}$ .

A considerable computational effort is required to determine the canonical expressions for quantities of types  $\Gamma_2, \Gamma_3, \dots$ . Consequently, we shall defer consideration of the problem of determining these expressions to a later date.

Generating Function:  $T$

$$GF(\Gamma_v) = \frac{Z_v}{(1-x)(1-x^2)^2(1-x^3)^2(1-x^4)}$$

3.3.13 Hextetrahedral class,  $T_d$  ,  $(\underline{I}, \underline{D}_1, \underline{D}_2, \underline{D}_3) \cdot (\underline{I}, \underline{M}_1, \underline{M}_2, \underline{I}_1, \underline{I}_2, \underline{I}_3)$

Gyroidal class,  $O$  ,  $(\underline{I}, \underline{D}_1, \underline{D}_2, \underline{D}_3) \cdot (\underline{I}, \underline{M}_1, \underline{M}_2)$ ,

$(\underline{C}, \underline{R}_1, \underline{R}_2, \underline{R}_3) \cdot (\underline{I}_1, \underline{I}_2, \underline{I}_3)$

Hexoctahedral class,  $O_h$  ,

$(\underline{I}, \underline{C}, \underline{R}_1, \underline{R}_2, \underline{R}_3, \underline{D}_1, \underline{D}_2, \underline{D}_3) \cdot (\underline{I}, \underline{M}_1, \underline{M}_2, \underline{I}_1, \underline{I}_2, \underline{I}_3)$

We observe that the general expressions for second-order tensor-valued functions  $T_{ij}(G_{kl})$  which are invariant under the group  $T_d$  , the group  $O$  or the group  $O_h$  are all identical. There are no vector-valued functions  $P_i(G_{kl})$  which are invariant under the group  $O$  or the group  $O_h$  . Hence, we restrict consideration to the group  $T_d$  . The matrices  $\underline{E}, \dots, \underline{H}$  appearing in Table 3.45 are defined in section 3.3.8. The matrices  $\underline{I}, \dots, \underline{R}_3 \underline{T}_3$  are defined in section 3.1. The notation  $\Sigma G_{11}, \dots$  employed below is defined in section 3.3.12.

Table 3.45 Irreducible Representations:  $T_d$

$T_d$	$\underline{I}$	$\underline{D}_1$	$\underline{D}_2$	$\underline{D}_3$	$\underline{M}_1$	$\underline{D}_1 \underline{M}_1$	$\underline{D}_2 \underline{M}_1$	$\underline{D}_3 \underline{M}_1$	$\underline{M}_2$	$\underline{D}_1 \underline{M}_2$	$\underline{D}_2 \underline{M}_2$	$\underline{D}_3 \underline{M}_2$
$\Gamma_1$	1	1	1	1	1	1	1	1	1	1	1	1
$\Gamma_2$	1	1	1	1	1	1	1	1	1	1	1	1
$\Gamma_3$	$\underline{E}$	$\underline{E}$	$\underline{E}$	$\underline{E}$	$\underline{A}$	$\underline{A}$	$\underline{A}$	$\underline{A}$	$\underline{B}$	$\underline{B}$	$\underline{B}$	$\underline{B}$
$\Gamma_4$	$\underline{I}$	$\underline{D}_1$	$\underline{D}_2$	$\underline{D}_3$	$\underline{M}_1$	$\underline{D}_1 \underline{M}_1$	$\underline{D}_2 \underline{M}_1$	$\underline{D}_3 \underline{M}_1$	$\underline{M}_2$	$\underline{D}_1 \underline{M}_2$	$\underline{D}_2 \underline{M}_2$	$\underline{D}_3 \underline{M}_2$
$\Gamma_5$	$\underline{I}$	$\underline{D}_1$	$\underline{D}_2$	$\underline{D}_3$	$\underline{M}_1$	$\underline{D}_1 \underline{M}_1$	$\underline{D}_2 \underline{M}_1$	$\underline{D}_3 \underline{M}_1$	$\underline{M}_2$	$\underline{D}_1 \underline{M}_2$	$\underline{D}_2 \underline{M}_2$	$\underline{D}_3 \underline{M}_2$

(continued)

Table 3.45 Irreducible Representations:  $T_d$  (continued)

$T_d$	$\bar{1}_1$	$\bar{D}_1\bar{1}_1$	$\bar{D}_2\bar{1}_1$	$\bar{D}_3\bar{1}_1$	$\bar{1}_2$	$\bar{D}_1\bar{1}_2$	$\bar{D}_2\bar{1}_2$	$\bar{D}_3\bar{1}_2$	$\bar{1}_3$	$\bar{D}_1\bar{1}_3$	$\bar{D}_2\bar{1}_3$	$\bar{D}_3\bar{1}_3$
$\Gamma_1$	1	1	1	1	1	1	1	1	1	1	1	1
$\Gamma_2$	-1	-1	-1	-1	-1	-1	-1	-1	-1	-1	-1	-1
$\Gamma_3$	$\bar{F}$	$\bar{F}$	$\bar{F}$	$\bar{F}$	$\bar{H}$	$\bar{H}$	$\bar{H}$	$\bar{H}$	$\bar{G}$	$\bar{G}$	$\bar{G}$	$\bar{G}$
$\Gamma_4$	$\bar{1}_1$	$\bar{D}_1\bar{1}_1$	$\bar{D}_2\bar{1}_1$	$\bar{D}_3\bar{1}_1$	$\bar{1}_2$	$\bar{D}_1\bar{1}_2$	$\bar{D}_2\bar{1}_2$	$\bar{D}_3\bar{1}_2$	$\bar{1}_3$	$\bar{D}_1\bar{1}_3$	$\bar{D}_2\bar{1}_3$	$\bar{D}_3\bar{1}_3$
$\Gamma_5$	$\bar{CT}_1$	$\bar{R}_1\bar{1}_1$	$\bar{R}_2\bar{1}_1$	$\bar{R}_3\bar{1}_1$	$\bar{CT}_2$	$\bar{R}_1\bar{1}_2$	$\bar{R}_2\bar{1}_2$	$\bar{R}_3\bar{1}_2$	$\bar{CT}_3$	$\bar{R}_1\bar{1}_3$	$\bar{R}_2\bar{1}_3$	$\bar{R}_3\bar{1}_3$



Table 3.46 Hexoctahedral class,  $T_d$ 

I.R.	Basic Quantities		$Z_v$
$\Gamma_1$	$T_{11}+T_{22}+T_{33}$	$G_{11}+G_{22}+G_{33}$	$1+x^3+x^4+x^5+x^6+x^9$
$\Gamma_3$	$\begin{vmatrix} 2T_{11}-T_{22}-T_{33} \\ \sqrt{3}(T_{22}-T_{33}) \end{vmatrix}$	$\begin{vmatrix} 2G_{11}-G_{22}-G_{33} \\ \sqrt{3}(G_{22}-G_{33}) \end{vmatrix}$	$x+2x^2+x^3+2x^4+2x^5+x^6+2x^7+x^8$
$\Gamma_4$	$(T_{23}, T_{31}, T_{12})^T$ $(P_1, P_2, P_3)^T$	$(G_{23}, G_{31}, G_{12})^T$	$x+2x^2+3x^3+3x^4+3x^5+3x^6+2x^7+x^8$

I.R.	Canonical Expressions
$\Gamma_1$	$a_0 + a_1 L_1 + a_2 L_2 + a_3 L_3 + a_4 L_1^2 + a_5 L_2 L_3$
$\Gamma_3$	$\sum_{i=1}^5 b_i J_i + (b_6 L_1 + b_7 L_2) J_1 + (b_8 L_1 + b_9 L_2) J_2 + (b_{10} L_1 + b_{11} L_2) J_3 + b_{12} L_2 J_4$
$\Gamma_4$	$\sum_{i=1}^8 c_i R_i + (c_9 L_1 + c_{10} L_2 + c_{11} L_3) R_1 + (c_{12} L_1 + c_{13} L_3) R_2 + (c_{14} L_1 + c_{15} L_2 + c_{16} L_3) R_3 + c_{17} L_3 R_5 + c_{18} L_2 R_6$

Integrity Basis:  $T_d$ 

$$K_1, \dots, K_6 = \Sigma G_{11}, \Sigma G_{11} G_{22}, G_{11} G_{22} G_{33}, \Sigma G_{23}^2, \Sigma G_{23}^2 G_{31}^2, G_{23} G_{31} G_{12}$$

$$L_1 = \Sigma G_{11} (G_{31}^2 + G_{12}^2), L_2 = \Sigma G_{11} G_{31}^2 G_{12}^2, L_3 = \Sigma G_{23}^2 G_{22} G_{33}$$

Quantities of type  $\Gamma_3 : T_d$ 

$$J_1 = \begin{vmatrix} 2G_{11}-G_{22}-G_{33} \\ \sqrt{3}(G_{22}-G_{33}) \end{vmatrix}, J_2 = \begin{vmatrix} 2G_{23}^2-G_{31}^2-G_{12}^2 \\ \sqrt{3}(G_{31}^2-G_{12}^2) \end{vmatrix}, J_3 = \begin{vmatrix} 2G_{11}^2-G_{22}^2-G_{33}^2 \\ \sqrt{3}(G_{22}^2-G_{33}^2) \end{vmatrix}$$

$$J_4 = \begin{vmatrix} 2G_{11} G_{23}^2 - G_{22} G_{31}^2 - G_{33} G_{12}^2 \\ \sqrt{3}(G_{22} G_{31}^2 - G_{33} G_{12}^2) \end{vmatrix}, J_5 = \begin{vmatrix} 2G_{23}^4 - G_{31}^4 - G_{12}^4 \\ \sqrt{3}(G_{31}^4 - G_{12}^4) \end{vmatrix}$$

Quantities of type  $\Gamma_4 : T_d$

$$\tilde{R}_1 = \begin{vmatrix} G_{23} \\ G_{31} \\ G_{12} \end{vmatrix}, \quad \tilde{R}_2 = \begin{vmatrix} G_{31}G_{12} \\ G_{12}G_{23} \\ G_{23}G_{31} \end{vmatrix}, \quad \tilde{R}_3 = \begin{vmatrix} G_{11}G_{23} \\ G_{22}G_{31} \\ G_{33}G_{12} \end{vmatrix}, \quad \tilde{R}_4 = \begin{vmatrix} G_{23}^3 \\ G_{31}^3 \\ G_{12}^3 \end{vmatrix},$$

$$\tilde{R}_5 = \begin{vmatrix} G_{11}G_{31}G_{12} \\ G_{22}G_{12}G_{23} \\ G_{33}G_{23}G_{31} \end{vmatrix}, \quad \tilde{R}_6 = \begin{vmatrix} G_{22}G_{33}G_{23} \\ G_{33}G_{11}G_{31} \\ G_{11}G_{22}G_{12} \end{vmatrix}, \quad \tilde{R}_7 = \begin{vmatrix} G_{11}G_{23}^3 \\ G_{22}G_{31}^3 \\ G_{33}G_{12}^3 \end{vmatrix},$$

$$\tilde{R}_8 = \begin{vmatrix} G_{22}G_{33}G_{31}G_{12} \\ G_{33}G_{11}G_{12}G_{23} \\ G_{11}G_{22}G_{23}G_{31} \end{vmatrix}$$

Generating Function:  $T_d$

$$GF(\Gamma_v) = \frac{Z_v}{(1-x)(1-x^2)^2(1-x^3)^2(1-x^4)}$$

## 4. Function Bases

### 4.1 Introduction

Let  $W(\underline{S})$  denote a scalar-valued function of a symmetric second-order tensor  $\underline{S}$ . For example  $W(\underline{S})$  could be the strain-energy function and  $\underline{S}$  the strain tensor. If the material possesses symmetry properties defined by a group of transformations  $\{A\} = \{\underline{A}_1, \dots, \underline{A}_n\}$ , then there are restrictions imposed on the form of  $W(\underline{S})$ . Thus

$$W(\underline{S}) = W(\underline{A}\underline{S}\underline{A}^T) \quad (4.1.1)$$

for all  $\underline{A}$  belonging to the group  $\{A\}$ . The function  $W(\underline{S})$  which satisfies (4.1.1) is said to be invariant under  $\{A\}$ . We may determine a set of invariants  $I_j(\underline{S})$ ,  $j=1, \dots, n$ , which are polynomials in the components of  $\underline{S}$  such that any invariant  $W(\underline{S})$  which is a polynomial in the components of  $\underline{S}$  is expressible as a polynomial in the invariants  $I_j(\underline{S})$ ,  $j=1, \dots, n$ . The invariants  $I_j(\underline{S})$ ,  $j=1, \dots, n$  are said to form an integrity basis for polynomial functions  $W(\underline{S})$  invariant under  $\{A\}$ .

We are concerned with the problem of determining a set of invariants  $J_1(\underline{S}), \dots, J_m(\underline{S})$  ( $m \leq n$ ) such that any function  $W(\underline{S})$  which is invariant under a group  $\{A\}$  is expressible as a single-valued function of the invariants  $J_k(\underline{S})$ ,  $k=1, \dots, m$ . The invariants  $J_1, \dots, J_m$  are said to form a function basis for functions  $W(\underline{S})$  which are invariant under the group  $\{A\}$ .

In this section, we discuss methods which may be employed in determining function bases for scalar-valued functions  $W(\underline{S}_1, \underline{S}_2, \dots, \underline{S}_N)$  of  $N$  symmetric second-order tensors  $\underline{S}_1, \dots, \underline{S}_N$  which are invariant

under a given crystallographic group belonging to the cubic crystal system. We first restrict consideration to functions  $W(\underline{S})$  of a single tensor  $\underline{S}$ . The elements of the integrity basis for functions  $W(\underline{S})$  which are invariant under the cubic group designated by  $T$  are known [10] and we may denote these by  $I_1, \dots, I_{14}$ . These invariants are related by functions.

$$f(I_1, \dots, I_{14}) = 0 \quad , \quad g(I_1, I_2, \dots) = 0 \quad , \dots \quad (4.1.2)$$

which are not identically zero when considered as functions of the  $I_1, I_2, \dots$  but which are identically zero when the  $I_1, I_2, \dots$  are expressed in terms of the tensor  $\underline{S}$ . Such relations are referred to as syzygies. All syzygies relating the invariants  $I_1, I_2, \dots$  are consequences of the elements

$$K_1(I_1, I_2, \dots) = 0 \quad , \dots , \quad K_p(I_1, I_2, \dots) = 0 \quad (4.1.3)$$

of a syzygy basis. Thus, each of the syzygies (4.1.2) are such that

$$f(I_1, I_2, \dots) = \alpha_1 K_1(I_1, I_2, \dots) + \dots + \alpha_p K_p(I_1, I_2, \dots) \quad (4.1.4)$$

where the  $\alpha_1, \dots, \alpha_p$  are polynomials in the  $I_1, I_2, \dots$ . We then have at our disposal all of the relations relating the invariants  $I_1, I_2, \dots$ . We then may make use of these identities to show that the values of all of the elements of the integrity basis are always known when the values of a number of invariants  $J_1, \dots, J_m$  are known. The  $J_i, (i=1, \dots, m)$ , then form a function basis.

In order to assist with the task of determining the syzygy basis, we may compute the generating function  $GF(x)$  for the number of linearly independent invariants of degree  $n$  in  $\underline{S}$ .  $GF(x)$  is a rational function in  $x$  such that, when formally expanded as a polynomial, the coefficient of  $x^n$  in the expansion gives the number of linearly independent invariants of degree  $n$  in  $\underline{S}$ . Inspection of the generating function enables us to make an educated guess as to the number and degree of the elements of the syzygy basis.

This procedure is effective when considering the problem of determining function bases for functions  $W(\underline{S})$  of a single tensor. In more complicated cases, e.g. finding a function basis for  $W(\underline{S}_1, \underline{S}_2, \underline{S}_3)$ , the number of elements of the integrity basis is large and the problem of determining the syzygy basis can become very tedious. Further, even if we have a number of functions (syzygies) relating the elements of the integrity basis, it is not at all clear that these syzygies will be of much assistance in finding  $I_p, I_q, \dots$  of the integrity basis whose values are always determined by the values of the remaining elements of the integrity basis. Thus, in more complicated cases, another procedure outlined below is usually more efficient.

Consider the set of tensors

$$A_1 S A_1^T = \underline{S}, A_2 S A_2^T, \dots, A_n S A_n^T \quad (4.1.5)$$

where the components of the symmetric second-order tensor  $\underline{S}$  are specified. We say that the set of tensors (4.1.5) lies on the same orbit. The transformations of the group  $\{A\}$  when applied to the

tensors (4.1.5) permute the tensors among themselves but the set of tensors is unaltered. We observe from (4.1.1) that a function  $W(\underline{S})$  takes on the same value when the argument of  $W(\underline{S})$  is replaced by any of the  $n$  tensors (4.1.5). Consider a six dimensional space in which  $(S_{11}, S_{22}, S_{33}, S_{23}, S_{31}, S_{12})$  denotes a point. The  $n$  points

$$(A_{1j}^{(p)} A_{1k}^{(p)} S_{jk}, A_{2j}^{(p)} A_{2k}^{(p)} S_{jk}, \dots, A_{lj}^{(p)} A_{lk}^{(p)} S_{jk}), (p=1, \dots, n) \quad (4.1.6)$$

constitute an orbit. We consider the problem of determining a set of invariants  $J_i(\underline{S})$  ( $i=1, \dots, m$ ) such that solution of the equations

$$J_1(\underline{S}) = \alpha_1, \dots, J_m(\underline{S}) = \alpha_m \quad (4.1.7)$$

will yield one set of solutions

$$A_{11} S_{11}^T, \dots, A_{nn} S_{nn}^T \quad (4.1.8)$$

which define a single orbit for  $\underline{S}$ . It is known (see Wineman and Pipkin [11]) that the elements of the integrity basis will provide such a set of invariants. It is usually the case that a lesser number of invariants will suffice to always uniquely specify a single orbit. We may construct such a set of invariants. The argument leading to the set of invariants  $J_1, \dots, J_m$  can be very intricate. It is therefore useful to use a combination of these procedures to most conveniently arrive at the set  $J_1, \dots, J_m$ . We observe that if we can define the orbit, we have the values of the tensors  $A_{11} S_{11}^T, \dots, A_{nn} S_{nn}^T$  and

hence can compute the value of any single-valued invariant function  $W(\underline{S})$  for which of course  $W(\underline{A}_1 \underline{S} \underline{A}_1^T) = \dots = W(\underline{A}_n \underline{S} \underline{A}_n^T)$ .

The question arises as to the number of invariants  $J_1, \dots, J_m$  which are required to form a function basis. One approach which is employed is to show that if any of the invariants  $J_i (i=1, \dots, m)$  is omitted from the list of elements of the function basis, then the remaining invariants do not constitute function basis. The invariants  $J_1, \dots, J_m$  are then said to form an irreducible function basis. Pennisi and Travato have employed this technique to discuss the irreducibility of the function basis for isotropic functions of vectors, skew-symmetric second-order tensors and symmetric second-order tensors given by Smith [12] and Boehler [13]. It is noted in [14] that even if  $J_1, \dots, J_m$  is shown to be irreducible in the sense discussed above, this does not preclude the existence of a set of invariants  $K_1, \dots, K_q (q < m)$  which also forms a function basis. We observe that this is indeed the case. Thus we may exhibit a function basis which is "irreducible" and then exhibit another which contains fewer terms.

It has been shown by Burnside [15] that if  $W$  is a function of  $k$  quantities ( $k=6$  for  $W(\underline{S})$ ) then the function basis must be comprised of at least  $k$  elements  $I_1, \dots, I_k$ . Burnside [15] maintains that we may determine another invariant  $I_{k+1}$  such that the  $k+1$  invariants form a function basis. Burnside is not explicit on the point but we believe that he means that a specific set of invariants will suffice to determine a unique orbit except in certain singular cases. In these

cases, different sets of  $k+1$  invariants might be required. We find that in cases of any complexity, it is usual that the number of basis elements comprising the function bases is substantially larger than  $k+1$ .

We consider below the problem of determining function bases for functions of  $N$  symmetric second-order tensors  $\underline{S}_1, \dots, \underline{S}_N$  which are invariant under the crystallographic groups

$$(i) \quad T, T_h$$

$$(ii) \quad T_d, O, O_h$$

Since the second-order tensor  $\underline{S}$  satisfies  $\underline{C}\underline{S}\underline{C}^T = \underline{S}$  where  $\underline{C}$  is the central inversion, ( $\underline{C} = \text{diag}(-1, -1, -1)$ ), the problems posed for the groups  $T$  and  $T_h$  are identical as are the problems posed for the groups  $T_d$ ,  $O$  and  $O_h$ .



## 4.2 A Function Basis for the Group T

We consider the problem of determining a function basis for scalar-valued functions  $W(\underline{S}_1, \underline{S}_2, \dots, \underline{S}_N)$  of a number of symmetric second-order tensors  $\underline{S}_1 = \|S_{ij}^{(1)}\|$ ,  $\underline{S}_2 = \|S_{ij}^{(2)}\|$ , ... which are invariant under the cubic crystallographic group T. The group T is comprised of the twelve matrices

$$\{\underline{A}_1, \dots, \underline{A}_{12}\} = \{\underline{I}, \underline{D}_1, \underline{D}_2, \underline{D}_3, \underline{M}_1, \underline{D}_1 \underline{M}_1, \underline{D}_2 \underline{M}_1, \underline{D}_3 \underline{M}_1, \underline{M}_2, \underline{D}_1 \underline{M}_2, \underline{D}_2 \underline{M}_2, \underline{D}_3 \underline{M}_2\} \quad (4.2.1)$$

where

$$\begin{aligned} \underline{I} &= \text{diag}(1, 1, 1), \quad \underline{D}_1 = \text{diag}(1, -1, -1), \quad \underline{D}_2 = \text{diag}(-1, 1, -1), \\ \underline{D}_3 &= \text{diag}(-1, -1, 1), \end{aligned} \quad (4.2.2)$$

$$\underline{M}_1 = \begin{bmatrix} 0 & 1 & 0 \\ 0 & 0 & 1 \\ 1 & 0 & 0 \end{bmatrix}, \quad \underline{M}_2 = \begin{bmatrix} 0 & 0 & 1 \\ 1 & 0 & 0 \\ 0 & 1 & 0 \end{bmatrix}.$$

A function  $W(\underline{S}_1, \dots, \underline{S}_N)$  is invariant under the group T if  $W(\underline{S}_1, \dots, \underline{S}_N)$  is unaltered when the set of components  $(S_{11}, S_{22}, S_{33}, S_{23}, S_{31}, S_{12})$  of a typical tensor  $\underline{S}$  is replaced by any of the sets

$$\begin{aligned} &(S_{11}, S_{22}, S_{33}, S_{23}, S_{31}, S_{12}), (S_{11}, S_{22}, S_{33}, S_{23}, -S_{31}, -S_{12}), \\ &(S_{11}, S_{22}, S_{33}, -S_{23}, S_{31}, -S_{12}), (S_{11}, S_{22}, S_{33}, -S_{23}, -S_{31}, S_{12}), \\ &(S_{22}, S_{33}, S_{11}, S_{31}, S_{12}, S_{23}), (S_{22}, S_{33}, S_{11}, S_{31}, -S_{12}, -S_{23}), \\ &(S_{22}, S_{33}, S_{11}, -S_{31}, S_{12}, -S_{23}), (S_{22}, S_{33}, S_{11}, -S_{31}, -S_{12}, S_{23}), \\ &(S_{33}, S_{11}, S_{22}, S_{12}, S_{23}, S_{31}), (S_{33}, S_{11}, S_{22}, S_{12}, -S_{23}, -S_{31}), \\ &(S_{33}, S_{11}, S_{22}, -S_{12}, S_{23}, -S_{31}), (S_{33}, S_{11}, S_{22}, -S_{12}, -S_{23}, S_{31}). \end{aligned} \quad (4.2.3)$$

If we are given the values of the invariants

$$\Sigma S_{11}, \Sigma S_{11}S_{22}, S_{11}S_{22}S_{33}, \Sigma S_{11}S_{22}(S_{11}-S_{22}), \quad (4.2.4)$$

we may determine three sets of solutions for  $(S_{11}, S_{22}, S_{33})$  which are of the form

$$(S_{11}, S_{22}, S_{33}) = (\alpha_1, \alpha_2, \alpha_3), (\alpha_2, \alpha_3, \alpha_1), (\alpha_3, \alpha_1, \alpha_2) \quad (4.2.5)$$

In (4.2.4),  $S_{11}, \dots, S_{12}$  denote the components of a tensor  $\underline{S}$  chosen from  $\underline{S}_1, \dots, \underline{S}_N$ . The quantity  $\Sigma S_{i_1 j_1} \dots S_{i_n j_n}$  denotes the sum of the three quantities obtained by permuting the subscripts in the summand cyclically. For example,  $\Sigma S_{11}S_{22} = S_{11}S_{22} + S_{22}S_{33} + S_{33}S_{11}$ . We choose one of these solutions, e.g.  $(S_{11}, S_{22}, S_{33}) = (\alpha_1, \alpha_2, \alpha_3)$ .

Then, given the values of the invariants on the left of Table 4.1, we may determine the values of the quantities on the right of Table 4.1 provided that

$$\begin{vmatrix} 1 & 1 & 1 \\ S_{11} & S_{22} & S_{33} \\ S_{33}-S_{22} & S_{11}-S_{33} & S_{22}-S_{11} \end{vmatrix} = \Sigma (S_{11}-S_{22})^2 \neq 0 \quad (4.2.6)$$

The condition (4.2.6) requires that  $S_{11} = S_{22} = S_{33}$  does not hold.

Table 4.1

$\Sigma S_{11}^{(i)}, \Sigma S_{11} S_{11}^{(i)}, \Sigma S_{11} (S_{22}^{(i)} - S_{33}^{(i)})$	$S_{11}^{(i)}, S_{22}^{(i)}, S_{33}^{(i)}$
$\Sigma (S_{23}^{(i)})^2, \Sigma S_{11} (S_{23}^{(i)})^2,$ $\Sigma S_{11} \{ (S_{31}^{(i)})^2 - (S_{12}^{(i)})^2 \}$	$(S_{23}^{(i)})^2, (S_{31}^{(i)})^2, (S_{12}^{(i)})^2$
$\Sigma S_{23}^{(i)} S_{23}^{(j)}, \Sigma S_{11} S_{23}^{(i)} S_{23}^{(j)}$ $\Sigma S_{11} (S_{31}^{(i)} S_{31}^{(j)} - S_{12}^{(i)} S_{12}^{(j)})$	$S_{23}^{(i)} S_{23}^{(j)}, S_{31}^{(i)} S_{31}^{(j)}, S_{12}^{(i)} S_{12}^{(j)}$

In Table 4.1, the indices  $i, j$  take on the values  $1, \dots, N$  and  $i < j$  in the last line. Suppose that we are given the values of the  $(S_{11}, S_{22}, S_{33})$ , the values of the quantities on the right of Table 4.1 and the values of the invariants

$$\begin{aligned}
 & S_{23}^{(i)} S_{31}^{(i)} S_{12}^{(i)}, \quad (i=1, \dots, N) \\
 & \Sigma S_{23}^{(i)} S_{31}^{(i)} S_{12}^{(j)}, \quad (i, j=1, \dots, N; i \neq j), \\
 & \Sigma S_{23}^{(i)} (S_{31}^{(j)} S_{12}^{(k)} + S_{12}^{(j)} S_{31}^{(k)}) , \quad (i, j, k=1, \dots, N; i \neq j \neq k \neq i).
 \end{aligned} \tag{4.2.7}$$

It has been shown by Boehler [16] that these quantities form a function basis for functions  $W(\tilde{S}_1, \dots, \tilde{S}_N)$  which are invariant under the group  $(\tilde{I}, \tilde{D}_1, \tilde{D}_2, \tilde{D}_3)$ . Thus the values of the  $(S_{11}, S_{22}, S_{33})$ , the quantities in Table (4.1) and the quantities (4.2.7) enable us to specify a unique orbit for the group  $(\tilde{I}, \tilde{D}_1, \tilde{D}_2, \tilde{D}_3)$ . Thus, we may determine four solutions for  $(S_{11}^{(i)}, \dots, S_{12}^{(i)})$  of the form

$$\begin{aligned}
(S_{11}^{(i)}, S_{22}^{(i)}, S_{33}^{(i)}, S_{23}^{(i)}, S_{31}^{(i)}, S_{12}^{(i)}) &= (a_i, b_i, c_i, d_i, e_i, f_i) , \\
(a_i, b_i, c_i, d_i, -e_i, -f_i) , & (a_i, b_i, c_i, -d_i, e_i, -f_i) , \\
(a_i, b_i, c_i, -d_i, -e_i, f_i) . &
\end{aligned} \tag{4.2.8}$$

The points lie on the same orbit. If we had chosen a different set of values for  $(S_{11}, S_{22}, S_{33})$  from the sets (4.2.5), the solutions (4.2.8) would be different but would still lie on the same orbit as the points (4.2.8). Thus, the invariants employed above would serve to determine a unique orbit provided that there is a tensor  $\tilde{S}$  chosen from among  $\tilde{S}_1, \dots, \tilde{S}_N$  for which  $S_{11} = S_{22} = S_{33}$  does not hold.

We next consider the case where  $S_{11}^{(i)} = S_{22}^{(i)} = S_{33}^{(i)}$  holds for  $i=1, \dots, N$ . In this case, the values of  $S_{11}^{(i)}, S_{22}^{(i)}, S_{33}^{(i)}$  are given by  $\frac{1}{3} \Sigma S_{11}^{(i)}$ . We need only consider the problem of finding a function basis for functions  $W(S_{23}^{(i)}, S_{31}^{(i)}, S_{12}^{(i)})$  which are invariant under the group  $T$ . Let  $\tilde{S}$  denote some tensor chosen from the list  $\tilde{S}_1, \dots, \tilde{S}_N$ . Then given the values of the invariants

$$\Sigma S_{23}^2, \Sigma S_{23}^2 S_{31}^2, S_{23} S_{31} S_{12}, \Sigma S_{23}^2 S_{31}^2 (S_{23}^2 - S_{31}^2) , \tag{4.2.9}$$

we may determine three sets of values for  $(S_{23}^2, S_{31}^2, S_{12}^2)$ . Thus,

$$(S_{23}^2, S_{31}^2, S_{12}^2) = (\alpha_1, \alpha_2, \alpha_3), (\alpha_2, \alpha_3, \alpha_1), (\alpha_3, \alpha_1, \alpha_2) \tag{4.2.10}$$

Then, given the values of the invariants on the left of Table 4.2, we may determine the values of the quantities on the right of the table provided that

$$\begin{vmatrix} 1 & 1 & 1 \\ s_{23}^2 & s_{31}^2 & s_{12}^2 \\ s_{31}^2 - s_{12}^2 & s_{12}^2 - s_{23}^2 & s_{23}^2 - s_{31}^2 \end{vmatrix} = -\Sigma(s_{23}^2 - s_{31}^2)^2 \neq 0 . \quad (4.2.11)$$

The condition (4.2.11) requires that  $s_{23}^2 = s_{31}^2 = s_{12}^2$  does not hold.

Table 4.2

$\Sigma(s_{23}^{(i)})^2, \Sigma s_{23}^2 (s_{23}^{(i)})^2,$	$(s_{23}^{(i)})^2, (s_{31}^{(i)})^2, (s_{12}^{(i)})^2$
$\Sigma s_{23}^2 \{(s_{31}^{(i)})^2 - (s_{12}^{(i)})^2\}$	
$\Sigma s_{23}^{(i)} s_{23}^{(j)}, \Sigma s_{23}^2 s_{23}^{(i)} s_{23}^{(j)},$	$s_{23}^{(i)} s_{23}^{(j)}, s_{31}^{(i)} s_{31}^{(j)}, s_{12}^{(i)} s_{12}^{(j)}$
$\Sigma s_{23}^2 \{s_{31}^{(i)} s_{31}^{(j)} - s_{12}^{(i)} s_{12}^{(j)}\}$	

Given the values of the quantities on the right of Table 4.2 and the values of the invariants (4.2.7), we may employ the argument given above to show that we may determine four solutions to the equations  $(s_{23}^{(j)})^2 = \gamma_i, \dots, \Sigma s_{23}^{(i)} (s_{31}^{(j)} s_{12}^{(k)} + s_{12}^{(j)} s_{31}^{(k)}) = \tau_{ijk}$  of the form

$$(s_{23}^{(i)}, s_{31}^{(i)}, s_{12}^{(i)}) = (\beta_1^{(i)}, \beta_2^{(i)}, \beta_3^{(i)}), (\beta_1^{(i)}, -\beta_2^{(i)}, -\beta_3^{(i)}), \quad (4.2.12)$$

$$(-\beta_1^{(i)}, \beta_2^{(i)}, -\beta_3^{(i)}), (-\beta_1^{(i)}, -\beta_2^{(i)}, \beta_3^{(i)}) .$$

These points lie on the same orbit. Thus, given the values of the invariants  $\Sigma s_{11}^{(i)}, (i=1, \dots, N)$ , the invariants (4.2.7)

and the invariants in Table 4.2, we may determine a unique orbit for the case where  $S_{11}^{(i)} = S_{22}^{(i)} = S_{33}^{(i)}$  provided that (4.2.11) holds.

We next consider the case where  $(S_{23}^{(i)})^2 = (S_{31}^{(i)})^2 = (S_{12}^{(i)})^2$ . Given the value of  $S_{23}^{(i)} S_{31}^{(i)} S_{12}^{(i)}$ , we see that there are four possibilities,

$$\begin{aligned} (S_{23}^{(i)}, S_{31}^{(i)}, S_{12}^{(i)}) &= (\alpha_i, \alpha_i, \alpha_i), (\alpha_i, -\alpha_i, -\alpha_i), \\ &(-\alpha_i, \alpha_i, -\alpha_i), (-\alpha_i, -\alpha_i, \alpha_i). \end{aligned} \quad (4.2.13)$$

We choose one of the  $S_i$  for which  $\alpha_i \neq 0$ . Thus, suppose that  $\alpha_1 \neq 0$ . We then choose one of the four solutions, e.g.

$$(S_{23}^{(1)}, S_{31}^{(1)}, S_{12}^{(1)}) = (\alpha_1, \alpha_1, \alpha_1). \quad (4.2.14)$$

Then  $\Sigma S_{23}^{(1)} S_{23}^{(2)} = 3\alpha_1 \alpha_2$  or  $-\alpha_1 \alpha_2$ . If the first alternative obtains, we have

$$(S_{23}^{(1)}, S_{31}^{(1)}, S_{12}^{(1)}; S_{23}^{(2)}, S_{31}^{(2)}, S_{12}^{(2)}) = (\alpha_1, \alpha_1, \alpha_1; \alpha_2, \alpha_2, \alpha_2). \quad (4.2.15)$$

If the second alternative applies, we have three possibilities.

$$(S_{23}^{(1)}, S_{31}^{(1)}, S_{12}^{(1)}; S_{23}^{(2)}, S_{31}^{(2)}, S_{12}^{(2)}) = (\alpha_1, \alpha_1, \alpha_1; \alpha_2, -\alpha_2, -\alpha_2) \quad (4.2.16)$$

$$(\alpha_1, \alpha_1, \alpha_1; -\alpha_2, \alpha_2, -\alpha_2), (\alpha_1, \alpha_1, \alpha_1; -\alpha_2, -\alpha_2, \alpha_2).$$

These points however all lie on the same orbit. Suppose that (4.2.15) holds. Then given the value of  $\Sigma S_{23}^{(1)} S_{23}^{(3)}$ , we may determine either one or three solutions for  $(S_{23}^{(1)}, S_{31}^{(1)}, S_{12}^{(1)}; S_{23}^{(2)}, S_{31}^{(2)}, S_{12}^{(2)}; S_{23}^{(3)}, S_{31}^{(3)}, S_{12}^{(3)})$ .

$s_{23}^{(3)}, s_{31}^{(3)}, s_{12}^{(3)}$  . If the case that three solutions occur, the resulting points are again on the same orbit. Suppose now that (4.2.16) holds. We choose one of the solutions, e.g.

$$(s_{23}^{(1)}, s_{31}^{(1)}, s_{12}^{(1)}; s_{23}^{(2)}, s_{31}^{(2)}, s_{12}^{(2)}) = (\alpha_1, \alpha_1, \alpha_1; \alpha_2, -\alpha_2, -\alpha_2). \quad (4.2.17)$$

Then the points

$$\begin{aligned} & (s_{23}^{(1)}, s_{31}^{(1)}, s_{12}^{(1)} ; s_{23}^{(2)}, s_{31}^{(2)}, s_{12}^{(2)} ; s_{23}^{(3)}, s_{31}^{(3)}, s_{12}^{(3)}) = \\ & (\alpha_1, \alpha_1, \alpha_1 ; \alpha_2, -\alpha_2, -\alpha_2 ; \alpha_3, \alpha_3, \alpha_3) , \\ & (\alpha_1, \alpha_1, \alpha_1 ; \alpha_2, -\alpha_2, -\alpha_2 ; \alpha_3, -\alpha_3, -\alpha_3) , \\ & (\alpha_1, \alpha_1, \alpha_1 ; \alpha_2, -\alpha_2, -\alpha_2 ; -\alpha_3, \alpha_3, -\alpha_3) , \\ & (\alpha_1, \alpha_1, \alpha_1 ; \alpha_2, -\alpha_2, -\alpha_2 ; -\alpha_3, -\alpha_3, \alpha_3) \end{aligned} \quad (4.2.18)$$

may lie on four different orbits. The invariants  $\Sigma s_{23}^{(1)} s_{23}^{(3)}$  ,  $\Sigma s_{23}^{(2)} s_{23}^{(3)}$  ,  $\Sigma s_{23}^{(1)} (s_{31}^{(2)} s_{12}^{(3)} - s_{12}^{(2)} s_{31}^{(3)})$  take on the values

$$\begin{aligned} & (3\alpha_1\alpha_3 , -\alpha_2\alpha_3 , -2\alpha_1\alpha_2\alpha_3) , (-\alpha_1\alpha_3 , 3\alpha_2\alpha_3 , -2\alpha_1\alpha_2\alpha_3) , \\ & (-\alpha_1\alpha_3 , -\alpha_2\alpha_3 , 4\alpha_1\alpha_2\alpha_3) , (-\alpha_1\alpha_3 , -\alpha_2\alpha_3 , -4\alpha_1\alpha_2\alpha_3) \end{aligned} \quad (4.2.19)$$

respectively on the four orbits. Thus, we may determine which orbit is appropriate since the sets of values (4.2.19) are all different. Continuing in this fashion, we see that the orbit may always be

uniquely defined for the case (4.2.13) if we have available the values of the invariants  $\Sigma S_{23}^{(i)} S_{23}^{(j)}$ ,  $(i, j=1, \dots, N; 1 < j)$  and  $\Sigma S_{23}^{(i)} (S_{31}^{(j)} S_{12}^{(k)} - S_{12}^{(j)} S_{31}^{(k)})$ ,  $(i, j, k=1, \dots, N; i < j < k)$ .

The set of invariants employed above to determine a unique orbit for the  $S_1, \dots, S_N$  will form a function basis for functions  $W(S_1, \dots, S_N)$  invariant under the group  $T$ . We observe that this result may be sharpened. Thus, we have the identity

$$\begin{aligned} \Sigma S_{23}^2 \cdot \Sigma S_{23}^2 T_{23}^2 &= 2 \Sigma S_{23} T_{23} \cdot \Sigma S_{23}^3 T_{23} - \Sigma S_{23}^2 \cdot (\Sigma S_{23} T_{23})^2 + \\ &+ 2 \Sigma S_{23}^2 S_{31}^2 \cdot \Sigma T_{23}^2 - 2 (\Sigma S_{23} S_{31} T_{12})^2 + 6 S_{23} S_{31} S_{12} \cdot \Sigma T_{23} T_{31} S_{12}. \end{aligned} \quad (4.2.20)$$

The value of  $\Sigma S_{23}^2 T_{23}^2$  may be determined provided that the values of the invariants on the right of (4.2.17) are given and provided that  $\Sigma S_{23}^2 \neq 0$ . If  $\Sigma S_{23}^2 = 0$ , then  $S_{23}^2 = S_{31}^2 = S_{12}^2 = 0$  and hence  $\Sigma S_{23}^2 T_{23}^2 = 0$ . Hence  $\Sigma S_{23}^2 T_{23}^2$  need not be included in the list of invariants forming the function basis. Identities similar to (4.2.20) indicate that invariants of the form  $\Sigma S_{23}^2 T_{23} U_{23}$ ,  $\Sigma T_{23}^2 S_{23} U_{23}$ ,  $\Sigma U_{23}^2 S_{23} T_{23}$  are not required.

We further note that the values of the invariants

$$J_1 = \Sigma S_{11}, J_2 = \Sigma S_{11} S_{22}, J_3 = S_{11} S_{22} S_{33}, J_4 = \Sigma S_{11} S_{22} (S_{11} - S_{22}) \quad (4.2.21)$$

may be determined if the values of the invariants

$$J_1 = \Sigma S_{11}, J_5 = \Sigma S_{11} S_{22} (S_{11} + S_{22}), J_4 = \Sigma S_{11} S_{22} (S_{11} - S_{22}) \quad (4.2.22)$$



are given. Thus we have the identities

$$4(J_1^2 - 3J_2)^3 = (2J_1^3 - 9J_5)^2 + 27J_4^2$$

$$3J_3 = J_1J_2 - J_5$$

which enable us to determine the values of the invariants (4.2.21) given the values of the invariants (4.2.22) .

We also note that

$$\begin{aligned} \Sigma(S_{23}T_{31} - S_{31}T_{23})^2 \cdot \Sigma S_{23}(T_{31}U_{12} + T_{12}U_{31}) = \\ = \Sigma S_{23}U_{23}(2\Sigma S_{23}S_{31}T_{12}^3 - 2T_{23}T_{31}T_{12} \cdot \Sigma S_{23}^2) + \\ + \Sigma T_{23}U_{23}(2\Sigma T_{23}T_{31}S_{12}^3 - 2S_{23}S_{31}S_{12} \cdot \Sigma T_{23}^2) + \\ + \Sigma S_{23}(T_{31}U_{12} - T_{12}U_{23}) \cdot \Sigma(S_{23}^2T_{31}^2 - S_{31}^2T_{23}^2) . \end{aligned} \quad (4.2.24)$$

The identity (4.2.24) enables us to argue that the invariant  $\Sigma S_{23}(T_{31}U_{12} + T_{12}U_{31})$  need be included as an element of the function basis.

We now employ the following notation to denote the elements of a function basis for functions  $W(\underline{S}_1, \dots, \underline{S}_N)$  which are invariant under a crystallographic group.

1.  $L_1(\underline{S}), \dots, L_p(\underline{S})$  ;
2.  $M_1(\underline{S}, \underline{T}), \dots, M_q(\underline{S}, \underline{T})$  ;
3.  $N_1(\underline{S}, \underline{T}, \underline{U}), \dots, N_r(\underline{S}, \underline{T}, \underline{U})$  ;

(4.2.25)

The quantities on the first line of (4.2.25) represent the  $\binom{N}{1}$  set of quantities obtained from these by substituting  $\underline{S}_1, \dots, \underline{S}_N$  in turn for  $\underline{S}$ . The quantities on the second line of (4.2.25) represent the  $\binom{N}{2}$  sets of quantities obtained from these by substituting  $\underline{S}_i$  for  $\underline{S}$ ,  $\underline{S}_j$  for  $\underline{T}$  ( $i, j=1, \dots, N; i < j$ ). The quantities on the third line of (4.2.25) represent the  $\binom{N}{3}$  sets of quantities obtained from these by substituting  $\underline{S}_i$  for  $\underline{S}$ ,  $\underline{S}_j$  for  $\underline{T}$ ,  $\underline{S}_k$  for  $\underline{U}$  ( $i, j, k=1, \dots, N; i < j < k$ ).

We then see from the argument given above that, using the notation (4.2.25), a function basis for functions  $W(\underline{S}_1, \dots, \underline{S}_N)$  invariant under  $T$  is given by

$$\begin{aligned}
1. \quad & \Sigma S_{11}, \Sigma S_{11} S_{22} (S_{11} + S_{22}), \Sigma S_{11} S_{22} (S_{11} - S_{22}), \\
& \Sigma S_{23}^2, \Sigma S_{23}^2 S_{31}^2, S_{23} S_{31} S_{12}, \Sigma S_{23}^2 S_{31}^2 (S_{23}^2 - S_{31}^2), \\
& \Sigma S_{11} S_{23}^2, \Sigma S_{11} (S_{31}^2 - S_{12}^2) . \\
2. \quad & \Sigma S_{11} T_{11}, \Sigma S_{11} (T_{22} - T_{33}), \\
& \Sigma S_{23} T_{23}, \Sigma S_{23} S_{31} T_{12}, \Sigma T_{23} T_{31} S_{12}, \\
& \Sigma S_{23}^2 (T_{31}^2 - T_{12}^2), \Sigma S_{23}^3 T_{23}, \Sigma S_{23}^2 (S_{31} T_{31} - S_{12} T_{12}), \\
& \Sigma T_{23}^3 S_{23}, \Sigma T_{23}^2 (S_{31} T_{31} - S_{12} T_{12}), \Sigma T_{11} S_{23}^2, \\
& \Sigma S_{11} T_{23}^2, \Sigma S_{11} (T_{31}^2 - T_{12}^2), \Sigma T_{11} (S_{31}^2 - S_{12}^2), \\
& \Sigma S_{11} S_{23} T_{23}, \Sigma S_{11} (S_{31} T_{31} - S_{12} T_{12}), \Sigma T_{11} S_{23} T_{23}, \Sigma T_{11} (S_{31} T_{31} - S_{12} T_{12}) .
\end{aligned}
\tag{4.2.26}$$

(continued)

$$3. \quad \Sigma S_{23}(T_{31}U_{12}-T_{12}U_{31}),$$

$$\Sigma S_{11}T_{23}U_{23}, \quad \Sigma S_{11}(T_{31}U_{31}-T_{12}U_{12}), \quad \Sigma T_{11}S_{23}U_{23},$$

$$\Sigma T_{11}(S_{31}U_{31}-S_{12}U_{12}), \quad \Sigma U_{11}S_{23}T_{23}, \quad \Sigma U_{11}(S_{31}T_{31}-S_{12}T_{12}),$$

$$\Sigma S_{23}^2(T_{31}U_{31}-T_{12}U_{12}), \quad \Sigma T_{23}^2(S_{31}U_{31}-S_{12}U_{12}), \quad \Sigma U_{23}^2(S_{31}T_{31}-S_{12}T_{12}) \ .$$

(4.2.26)

### 4.3 A Function Basis for the Group $T_d$

We consider the problem of determining a function basis for scalar-valued functions  $W(\underline{S}_1, \underline{S}_2, \dots, \underline{S}_N)$  of a number of symmetric second-order tensors  $\underline{S}_1 = \|S_{ij}^{(1)}\|$ ,  $\underline{S}_2 = \|S_{ij}^{(2)}\|$ , ... which are invariant under the crystallographic group  $T_d$ . The group  $T_d$  is comprised of the twenty-four matrices

$$\begin{aligned} \{A_1, \dots, A_{24}\} = & (I, D_1, D_2, D_3, M_1, D_1 M_1, D_2 M_1, D_3 M_1, M_2, D_1 M_2, D_2 M_2, D_3 M_2, \\ & T_1, D_1 T_1, D_2 T_1, D_3 T_1, T_2, D_1 T_2, D_2 T_2, D_3 T_2, T_3, D_1 T_3, \\ & D_2 T_3, D_3 T_3) \end{aligned} \quad (4.3.1)$$

where the matrices  $I, D_1, D_2, D_3, M_1, M_2$  are defined by (4.2.2) and where

$$T_1 = \begin{vmatrix} 1 & 0 & 0 \\ 0 & 0 & 1 \\ 0 & 1 & 0 \end{vmatrix}, \quad T_2 = \begin{vmatrix} 0 & 0 & 1 \\ 0 & 1 & 0 \\ 1 & 0 & 0 \end{vmatrix}, \quad T_3 = \begin{vmatrix} 0 & 1 & 0 \\ 1 & 0 & 0 \\ 0 & 0 & 1 \end{vmatrix}. \quad (4.3.2)$$

A function  $W(\underline{S}_1, \dots, \underline{S}_N)$  is invariant under the group  $T_d$  if  $W(\underline{S}_1, \dots, \underline{S}_N)$  is unaltered when the set of components  $(S_{11}, S_{22}, S_{33}, S_{23}, S_{31}, S_{12})$  of a typical tensor  $\underline{S}$  are replaced by any of the sets

$$\begin{aligned} & (S_{11}, S_{22}, S_{33}, S_{23}, S_{31}, S_{12}), (S_{11}, S_{22}, S_{33}, S_{23}, -S_{31}, -S_{12}), \\ & (S_{11}, S_{22}, S_{33}, -S_{23}, S_{31}, -S_{12}), (S_{11}, S_{22}, S_{33}, -S_{23}, -S_{31}, S_{12}), \\ & (S_{22}, S_{33}, S_{11}, S_{31}, S_{12}, S_{23}), (S_{22}, S_{33}, S_{11}, S_{31}, -S_{12}, -S_{23}), \\ & (S_{22}, S_{33}, S_{11}, -S_{31}, S_{12}, -S_{23}), (S_{22}, S_{33}, S_{11}, -S_{31}, -S_{12}, S_{23}), \\ & \text{(continued)} \end{aligned} \quad (4.3.3)$$

$$\begin{aligned}
& (S_{33}, S_{11}, S_{22}, S_{12}, S_{23}, S_{31}) , (S_{33}, S_{11}, S_{22}, S_{12}, -S_{23}, -S_{31}) , \\
& (S_{33}, S_{11}, S_{22}, -S_{12}, S_{23}, -S_{31}) , (S_{33}, S_{11}, S_{22}, -S_{12}, -S_{23}, S_{31}) , \\
& (S_{22}, S_{11}, S_{33}, S_{31}, S_{23}, S_{12}) , (S_{22}, S_{11}, S_{33}, S_{31}, -S_{23}, -S_{12}) , \\
& (S_{22}, S_{11}, S_{33}, -S_{31}, S_{23}, -S_{12}) , (S_{22}, S_{11}, S_{33}, -S_{31}, -S_{23}, S_{12}) , \\
& (S_{33}, S_{22}, S_{11}, S_{12}, S_{31}, S_{23}) , (S_{33}, S_{22}, S_{11}, S_{12}, -S_{31}, -S_{23}) , \\
& (S_{33}, S_{22}, S_{11}, -S_{12}, S_{31}, -S_{23}) , (S_{33}, S_{22}, S_{11}, -S_{12}, -S_{31}, S_{23}) , \\
& (S_{11}, S_{33}, S_{22}, S_{23}, S_{12}, S_{31}) , (S_{11}, S_{33}, S_{22}, S_{23}, -S_{12}, -S_{31}) , \\
& (S_{11}, S_{33}, S_{22}, -S_{23}, S_{12}, -S_{31}) , (S_{11}, S_{33}, S_{22}, -S_{23}, -S_{12}, S_{31}) .
\end{aligned}
\tag{4.3.3}$$

We first consider the problem of determining the elements of a function basis for  $W(\underline{S}_1, \dots, \underline{S}_N)$  which involve only diagonal components of the tensors  $\underline{S}_1, \dots, \underline{S}_N$ . Since the elements of an integrity basis form a function basis, we see from [17] that the elements of a function basis for functions of  $\underline{S}_1, \dots, \underline{S}_N$  which involve only diagonal components of the tensors  $\underline{S}_1, \dots, \underline{S}_N$  is given by

$$\begin{aligned}
1. & \quad \Sigma S_{11} , \Sigma S_{11}^2 , \Sigma S_{11}^3 . \\
2. & \quad \Sigma S_{11} T_{11} , \Sigma S_{11}^2 T_{11} , \Sigma T_{11}^2 S_{11} . \\
3. & \quad \Sigma S_{11} T_{11} U_{11} .
\end{aligned}
\tag{4.3.4}$$

In (4.3.4), we have employed the notation introduced in (4.2.25). We observe that the invariant  $\Sigma S_{11} T_{11} U_{11}$  satisfies the relation

$$\begin{aligned}
(I_1^2 - 3I_2)\Sigma S_{11}T_{11}U_{11} &= (I_1I_2 - I_3)(K_1I_4 - 3K_3) + I_1(I_1^2 - I_2)K_2 + \\
&+ (2K_3 - I_1K_1)(I_1J_1 - J_2) + (2J_1 - I_1I_4)(I_1K_3 - K_4) - \\
&- K_3J_2 - K_4J_1
\end{aligned} \tag{4.3.5}$$

where

$$\begin{aligned}
I_1 &= \Sigma S_{11}, \quad I_2 = \Sigma S_{11}^2, \quad I_3 = \Sigma S_{11}^3, \quad I_4 = \Sigma T_{11}, \quad K_1 = \Sigma U_{11}, \\
K_2 &= \Sigma T_{11}U_{11}, \quad K_3 = \Sigma S_{11}U_{11}, \quad K_4 = \Sigma S_{11}^2U_{11}, \quad J_1 = \Sigma S_{11}T_{11}, \\
J_2 &= \Sigma S_{11}^2T_{11}.
\end{aligned} \tag{4.3.6}$$

Thus, the value of the invariant  $\Sigma S_{11}T_{11}U_{11}$  is known once the values of the invariants (4.3.6) are known provided that  $I_1^2 - 3I_2 = -\Sigma(S_{11} - S_{22})^2 \neq 0$ . This could only happen if  $S_{11} = S_{22} = S_{33}$ . In this case,  $\Sigma S_{11}T_{11}U_{11} = \frac{1}{3} \Sigma S_{11} \cdot \Sigma T_{11}U_{11}$ . Hence we need not include  $\Sigma S_{11}T_{11}U_{11}$  as a basis element. Further, upon setting  $U_{11} = T_{11}$  in (4.3.5), we see that the resulting syzygy enables us to conclude that we may also eliminate  $\Sigma T_{11}^2 S_{11}$  from the function basis.

We next consider the problem of determining the elements of a function basis for  $W(\underline{S}_1, \dots, \underline{S}_N)$  which involve only off-diagonal components of the tensors  $\underline{S}_1, \dots, \underline{S}_N$ . Since the elements of an integrity basis form a function basis, we see from [17] that the elements of a

function basis which involve only off-diagonal components of the tensors is given by

1.  $\Sigma S_{23}^2$  ,  $\Sigma S_{23}^2 S_{31}^2$  ,  $S_{23} S_{31} S_{12}$  .
2.  $\Sigma S_{23} T_{23}$  ,  $\Sigma S_{23} S_{31} T_{12}$  ,  $\Sigma T_{23} T_{31} S_{12}$  ,  $\Sigma S_{23}^2 T_{23}^2$  ,  
 $\Sigma S_{23}^3 T_{23}$  ,  $\Sigma T_{23}^3 S_{23}$  . (4.3.7)
3.  $\Sigma S_{23}^2 T_{23} U_{23}$  ,  $\Sigma T_{23}^2 S_{23} U_{23}$  ,  $\Sigma U_{23}^2 S_{23} T_{23}$  ,  $\Sigma S_{23} (T_{31} U_{12} + T_{12} U_{31})$  .
4.  $\Sigma S_{23} T_{23} U_{23} V_{23}$  .

The notation given in (4.2.25) is again employed in (4.3.7). We may employ the argument given in section 4.2 (see eqn. (4.2.17) and the following discussion) to show that the invariants  $\Sigma S_{23}^2 T_{23}^2$  ,  $\Sigma S_{23}^2 T_{23} U_{23}$  ,  $\Sigma T_{23}^2 S_{23} U_{23}$  ,  $\Sigma U_{23}^2 S_{23} T_{23}$  and  $\Sigma S_{23} T_{23} U_{23} V_{23}$  are not required as elements of a function basis.

Thus, given the values of the invariants listed above, we may specify a single orbit for the diagonal components which consists of six sets of values for the quantities  $S_{11}, S_{22}, \dots$  given by

$$\begin{aligned}
 (S_{11}, S_{22}, S_{33}, T_{11}, T_{22}, T_{33}, U_{11}, U_{22}, U_{33}, \dots) = \\
 (\alpha_1, \alpha_2, \alpha_3, \beta_1, \beta_2, \beta_3, \gamma_1, \gamma_2, \gamma_3, \dots) , \\
 (\alpha_2, \alpha_3, \alpha_1, \beta_2, \beta_3, \beta_1, \gamma_2, \gamma_3, \gamma_1, \dots) , \dots , \\
 (\alpha_2, \alpha_1, \alpha_3, \beta_2, \beta_1, \beta_3, \gamma_2, \gamma_1, \gamma_3, \dots)
 \end{aligned}
 \tag{4.3.8}$$

and a single orbit for the off-diagonal components which consists of

twenty four sets of values for the quantities  $S_{23}, S_{31}, \dots$  given by

$$\begin{aligned}
 (S_{23}, S_{31}, S_{12}, T_{23}, T_{31}, T_{12}, U_{23}, U_{31}, U_{12}, \dots) = \\
 (a_1, a_2, a_3, b_1, b_2, b_3, c_1, c_2, c_3, \dots) , \\
 (a_1, -a_2, -a_3, b_1, -b_2, -b_3, c_1, -c_2, -c_3, \dots) , \dots, \\
 (-a_2, -a_1, a_3, -b_2, -b_1, b_3, -c_2, -c_1, c_3, \dots) .
 \end{aligned} \tag{4.3.9}$$

There are then twenty-four orbits which may be obtained by associating one set of values from (4.3.8) with any of twenty-four sets from (4.3.9). Of these, only six orbits would be distinct. We need the values of invariants involving both diagonal and off-diagonal components to determine which of the six orbits is appropriate.

Let us choose one of the sets of values (4.3.8) of the diagonal components, e.g.

$$\begin{aligned}
 (S_{11}, S_{22}, S_{33}, T_{11}, T_{22}, T_{33}, U_{11}, U_{22}, U_{33}, \dots) = \\
 (\alpha_1, \alpha_2, \alpha_3, \beta_1, \beta_2, \beta_3, \gamma_1, \gamma_2, \gamma_3, \dots) .
 \end{aligned} \tag{4.3.10}$$

Suppose there is a tensor  $\underline{S}$  among the  $\underline{S}_1, \dots, \underline{S}_N$  for which  $S_{11} \neq S_{22} \neq S_{33} \neq S_{11}$ . Further suppose that we are given the values of the invariants

$$\begin{aligned}
 \Sigma (S_{23}^{(i)})^2 , \Sigma S_{11} (S_{23}^{(i)})^2 , \Sigma S_{11}^2 (S_{23}^{(i)})^2 , (i=1, \dots, N) , \\
 \Sigma S_{23}^{(i)} S_{23}^{(j)} , \Sigma S_{11} S_{23}^{(i)} S_{23}^{(j)} , \Sigma S_{11}^2 S_{23}^{(i)} S_{23}^{(j)} , (i, j=1, \dots, N; i < j) .
 \end{aligned} \tag{4.3.11}$$



We may then determine the values of the quantities

$$(s_{23}^{(i)})^2, (s_{31}^{(i)})^2, (s_{12}^{(i)})^2, (i=1, \dots, N), \quad (4.3.12)$$

$$s_{23}^{(i)} s_{23}^{(j)}, s_{31}^{(i)} s_{31}^{(j)}, s_{12}^{(i)} s_{12}^{(j)}, (i, j=1, \dots, N; i < j).$$

provided that

$$\begin{vmatrix} 1 & 1 & 1 \\ s_{11} & s_{22} & s_{33} \\ s_{11}^2 & s_{22}^2 & s_{33}^2 \end{vmatrix} = (s_{11} - s_{22})(s_{22} - s_{33})(s_{33} - s_{11}) \neq 0. \quad (4.3.13)$$

Given the values of the quantities (4.3.12) and the values of the invariants

$$\begin{aligned} & s_{23}^{(i)} s_{31}^{(i)} s_{12}^{(i)}, (i=1, \dots, N), \\ & \Sigma s_{23}^{(i)} s_{31}^{(i)} s_{12}^{(j)}, (i, j=1, \dots, N; i \neq j), \\ & \Sigma s_{23}^{(i)} (s_{31}^{(j)} s_{12}^{(k)} + s_{12}^{(j)} s_{31}^{(k)}), (i, j, k = 1, \dots, N; i < j < k), \end{aligned} \quad (4.3.14)$$

we may employ the result of Boehler [16] and argue as in section 4.2 that we may determine four sets of solutions for the quantities  $s_{23}^{(i)}, s_{31}^{(i)}, s_{12}^{(i)}, (i=1, \dots, N)$ . This will suffice to determine which of the six possible orbits arises.

Suppose there is no tensor  $\underline{S}$  from the set  $\underline{S}_1, \dots, \underline{S}_N$  for which (4.3.13) holds. Suppose that there are two tensors  $\underline{S}$  and  $\underline{T}$  for which

$$S_{11}=S_{22}\neq S_{33} \quad , \quad T_{11}=T_{33}\neq T_{22} \quad . \quad (4.3.15)$$

Then, given the values of the invariants

$$\begin{aligned} & \Sigma (S_{23}^{(i)})^2 \quad , \quad \Sigma S_{11} (S_{23}^{(i)})^2 \quad , \quad \Sigma T_{11} (S_{23}^{(i)})^2 \quad , \quad (i=1, \dots, N) \quad , \\ & \Sigma S_{23}^{(i)} S_{23}^{(j)} \quad , \quad \Sigma S_{11} S_{23}^{(i)} S_{23}^{(j)} \quad , \quad \Sigma T_{11} S_{23}^{(i)} S_{23}^{(j)} \quad , \quad (i, j=1, \dots, N; \quad 1 < j) \quad , \end{aligned} \quad (4.3.16)$$

we may determine the values of the quantities (4.3.12) provided that

$$\begin{vmatrix} 1 & 1 & 1 \\ S_{11} & S_{11} & S_{33} \\ T_{11} & T_{22} & T_{11} \end{vmatrix} = (S_{11}-S_{33})(T_{22}-T_{11}) \neq 0 \quad . \quad (4.3.17)$$

In (4.3.17), we have employed the assumption that (4.3.15) is the case so that (4.3.17) of course holds. Then given the values of the quantities (4.3.12) and the values of the invariants (4.3.14), we may argue exactly as above that we may determine which of the six possible orbits applies.

We must still consider the case where the same pair of diagonal components is equal for all of the tensors  $\underline{S}_1, \dots, \underline{S}_N$ . Thus, we might have

$$S_{11}=S_{22}\neq S_{33} \quad , \quad T_{11}=T_{22}\neq T_{33} \quad , \quad U_{11}=U_{22}\neq U_{33} \quad , \dots \quad . \quad (4.3.18)$$

We leave this case until later. We note that if all diagonal components of a tensor  $\underline{S}$  are equal, i.e. if  $S_{11}=S_{22}=S_{33}$ , then  $S_{11} = \frac{1}{3} \Sigma S_{11} \quad , \dots \quad , \quad S_{33} = \frac{1}{3} \Sigma S_{33}$ . Hence the function basis for

functions  $W(S_{11}, S_{22}, S_{33}, S_{23}, S_{31}, S_{12}, T_{11}, T_{22}, T_{33}, \dots, U_{23}, U_{31}, U_{12}, \dots)$  is given by  $\Sigma S_{11}$  and a function basis for functions of  $W(S_{23}, S_{31}, S_{12}, T_{11}, T_{22}, T_{33}, \dots, U_{23}, U_{31}, U_{12}, \dots)$ . Thus, if we have a case where  $S_{11} = S_{22} = S_{33}$ , we may essentially ignore the variables  $S_{11}, S_{22}, S_{33}$ .

We have observed above that given the values of the invariants represented by

1.  $\Sigma S_{23}^2, \Sigma S_{23}^2 S_{31}^2, \Sigma S_{12} S_{23} S_{31}$ .
2.  $\Sigma S_{23} T_{23}, \Sigma S_{23} S_{31} T_{12}, \Sigma T_{23} T_{31} S_{12}, \Sigma S_{23}^3 T_{23}, \Sigma T_{23}^3 S_{23}$ . (4.3.19)
3.  $\Sigma S_{23} (T_{31} U_{12} + T_{12} U_{31})$

we may determine a single set of twenty-four solutions for the quantities  $(S_{23}, S_{31}, S_{12}, T_{23}, T_{31}, T_{12}, U_{23}, U_{31}, U_{12}, \dots)$ . Thus, we have

$$\begin{aligned}
 (S_{23}, S_{31}, S_{12}, T_{23}, T_{31}, T_{12}, U_{23}, U_{31}, U_{12}, \dots) = \\
 (\alpha_1, \alpha_2, \alpha_3, \beta_1, \beta_2, \beta_3, \gamma_1, \gamma_2, \gamma_3, \dots), \\
 (\alpha_1, -\alpha_2, -\alpha_3, \beta_1, -\beta_2, -\beta_3, \gamma_1, -\gamma_2, -\gamma_3, \dots), \\
 (-\alpha_1, \alpha_2, -\alpha_3, -\beta_1, \beta_2, -\beta_3, -\gamma_1, \gamma_2, -\gamma_3, \dots), \dots
 \end{aligned} \tag{4.3.20}$$

where there are twenty-four points in  $3N$  space on the right of (4.3.20). Suppose we choose one of the sets of values in (4.3.20), e.g. the first set. Then given the values of the  $S_{23}, S_{31}, \dots$  from (4.3.20) and the values of the invariants

$$\sum S_{11}^{(i)}, \sum S_{11}^{(i)} S_{23}^2, \sum S_{11}^{(i)} S_{23}^4 \quad (4.3.21)$$

where  $\underline{S}$  is some tensor chosen from  $\underline{S}_1, \dots, \underline{S}_N$ , we may determine the values of  $S_{11}^{(i)}, S_{22}^{(i)}, S_{33}^{(i)}$ ,  $(i=1, \dots, N)$  provided that

$$\begin{vmatrix} 1 & 1 & 1 \\ S_{23}^2 & S_{31}^2 & S_{12}^2 \\ S_{23}^4 & S_{31}^4 & S_{12}^4 \end{vmatrix} = (S_{23}^2 - S_{31}^2)(S_{31}^2 - S_{12}^2)(S_{12}^2 - S_{23}^2) \neq 0. \quad (4.3.22)$$

Suppose there is no tensor  $\underline{S}$  among the  $\underline{S}_1, \dots, \underline{S}_N$  for which  $S_{23}^2 \neq S_{31}^2 \neq S_{12}^2 \neq S_{23}^2$ . Suppose we have two tensors  $\underline{S}, \underline{T}$  for which

$$S_{23}^2 = S_{31}^2 \neq S_{12}^2, \quad T_{23}^2 = T_{12}^2 \neq T_{31}^2. \quad (4.3.23)$$

Then, given the values of the quantities (4.3.23) and the values of the invariants

$$\sum S_{11}^{(i)}, \sum S_{11}^{(i)} S_{23}^2, \sum S_{11}^{(i)} T_{23}^2, \quad (4.3.24)$$

we may determine the values of the quantities  $S_{11}^{(i)}, S_{22}^{(i)}, S_{33}^{(i)}$ ,  $(i=1, \dots, N)$  since

$$\begin{vmatrix} 1 & 1 & 1 \\ S_{23}^2 & S_{23}^2 & S_{12}^2 \\ T_{23}^2 & T_{31}^2 & T_{23}^2 \end{vmatrix} = (S_{12}^2 - S_{23}^2)(T_{31}^2 - T_{23}^2) = 0. \quad (4.3.25)$$

Suppose that, for all of the tensors  $\underline{S}_1, \dots, \underline{S}_N$ , we have

$$(S_{23}^{(i)})^2 = (S_{31}^{(i)})^2 \neq (S_{12}^{(i)})^2 \quad (4.3.26)$$

Let  $\underline{S}$  and  $\underline{T}$  be two tensors chosen from  $\underline{S}_1, \dots, \underline{S}_N$ . Suppose that

$$(S_{23}, S_{31}, S_{12}; T_{23}, T_{31}, T_{12}) = (\alpha_1, \alpha_1, \beta_1; \alpha_2, -\alpha_2, \beta_2) . \quad (4.3.27)$$

where  $\alpha_1^2 \neq \beta_1^2$ ,  $\alpha_2^2 \neq \beta_2^2$ . Then given the values of the quantities (4.3.27) and the values of the invariants

$$\Sigma S_{11}^{(i)}, \Sigma S_{11}^{(i)} S_{23}^2, \Sigma S_{11}^{(i)} S_{23} T_{23}, \quad (4.3.28)$$

we may determine the values of  $S_{11}^{(i)}, S_{22}^{(i)}, S_{33}^{(i)}$ , ( $i=1, \dots, N$ ) since from (4.3.27)

$$\begin{vmatrix} 1 & 1 & 1 \\ S_{23}^2 & S_{31}^2 & S_{12}^2 \\ S_{23}T_{23} & S_{31}T_{31} & S_{12}T_{12} \end{vmatrix} = 2(\beta_1^2 - \alpha_1^2)\alpha_1\alpha_2 \quad (4.3.29)$$

provided of course the  $\alpha_1 \neq 0$ ,  $\alpha_2 \neq 0$ . Suppose again that (4.3.26) holds but that there are not two of the  $\underline{S}_1, \dots, \underline{S}_N$  which may be chosen so that (4.3.27) is the case. Thus, we may have

$$(S_{23}, S_{31}, S_{12}; T_{23}, T_{31}, T_{12}; U_{23}, U_{31}, U_{12}; \dots) = \quad (4.3.30)$$

$$(\alpha_1, \alpha_1, \beta_1; \alpha_2, \alpha_2, \beta_2; \alpha_3, \alpha_3, \beta_3; \dots)$$

We have seen above that we were able to determine a function basis unless the diagonal components of  $\underline{S}_1, \dots, \underline{S}_N$  were such that one of

the three cases listed below obtains.

$$\begin{aligned}
 (S_{11}, S_{22}, S_{33}; T_{11}, T_{22}, T_{33}; U_{11}, U_{22}, U_{33}, \dots) = \\
 (a_1, a_1, b_1; a_2, a_2, b_2; a_3, a_3, b_3; \dots) \text{ or} \\
 (a_1, b_1, a_1; a_2, b_2, a_2; a_3, b_3, a_3; \dots) \text{ or} \\
 (b_1, a_1, a_1; b_2, a_2, a_2; b_3, a_3, a_3; \dots)
 \end{aligned} \tag{4.3.31}$$

If we combine the terms  $(S_{11}, S_{22}, S_{33}, T_{11}, \dots)$  and  $(S_{23}, S_{31}, S_{12}, T_{23}, \dots)$  and consider the resultant as a point in  $6N$  dimensional space, we observe that the set  $(4.3.30)$ ,  $(4.3.31)_2$  and  $(4.3.30)$ ,  $(4.3.31)_3$  lie on the same orbit whereas  $(4.3.30)$ ,  $(4.3.31)_1$  lies on a different orbit. The invariant  $\Sigma S_{11} S_{23}^2$  takes on the values

$$(a_1 + b_1)\alpha_1^2 + a_1\beta_1^2, \quad 2a_1\alpha_1^2 + b_1\beta_1^2 \tag{4.3.32}$$

respectively on the two orbits. These two values are different unless  $(a_1 - b_1)(\alpha_1^2 - \beta_1^2) = 0$ . Since this is not the case, the invariant  $\Sigma S_{11} S_{23}^2$  serves to distinguish between the two possible orbits. Thus, we would be able to specify a single orbit.

We still need to consider the case where  $(S_{23}^{(i)})^2 = (S_{31}^{(i)})^2 = (S_{12}^{(i)})^2$ ,  $(i=1, \dots, N)$ . Arguing in the same fashion as above, we would find that the values of the invariants of the form  $\Sigma S_{11} T_{23} U_{23}$  would suffice to distinguish between orbits for the case where the diagonal components are of the form (4.3.31).

We note that invariants of the form  $\Sigma T_{11} S_{23}^4$  which appear in (4.3.21) are not needed as elements of a function basis. Thus, we have an identity given by

$$\begin{aligned}
\frac{1}{2} \Sigma (T_{11} - T_{22})^2 \cdot \Sigma T_{11} S_{23}^4 &= 9 T_{11} T_{22} T_{33} \cdot \Sigma S_{23}^2 S_{31}^2 \\
&+ 3 \Sigma T_{11} S_{23}^2 \cdot \Sigma T_{11}^2 S_{23}^2 + \Sigma T_{11} \cdot \Sigma T_{11} \cdot \Sigma S_{23}^2 \cdot \Sigma T_{11} S_{23}^2 \\
&- \Sigma T_{11} \cdot \Sigma S_{23}^2 \cdot \Sigma T_{11}^2 S_{23}^2 - 2 \Sigma T_{11} \cdot (\Sigma T_{11} S_{23}^2)^2 \\
&- \Sigma T_{11} \cdot \Sigma T_{11} T_{22} \cdot \Sigma S_{23}^2 S_{31}^2 - 3 T_{11} T_{22} T_{33} \cdot (\Sigma S_{23}^2)^2 .
\end{aligned} \tag{4.3.33}$$

Thus the value of  $\Sigma T_{11} S_{23}^4$  is given once the value of the invariants  $\Sigma (T_{11} - T_{22})^2$  and the invariants on the right of (4.3.33) are given unless  $\Sigma (T_{11} - T_{22})^2 = 0$ . This would require that  $T_{11} = T_{22} = T_{33}$ . In this case the value of  $\Sigma T_{11} S_{23}^4$  is given by the value of  $\frac{1}{3} \Sigma T_{11} \cdot \Sigma S_{23}^4$ . Hence,  $\Sigma T_{11} S_{23}^4$  need not be included in a function basis.

Then, employing the notation (4.2.25) and the argument given above, we see that a function basis for functions  $W(\underline{S}_1, \dots, \underline{S}_N)$  invariant under the group  $T_d$  is given by

$$\begin{aligned}
1. \quad &\Sigma S_{11}, \Sigma S_{11}^2, \Sigma S_{11}^3, \Sigma S_{23}^2, \Sigma S_{23}^2 S_{31}^2, S_{23} S_{31} S_{12}, \Sigma S_{11} S_{23}^2, \\
&\Sigma S_{11}^2 S_{23}^2 .
\end{aligned} \tag{4.3.34}$$

(Continued)

$$\begin{aligned}
2. \quad & \Sigma S_{11} T_{11} , \Sigma S_{11}^2 T_{11} , \Sigma S_{23} T_{23} , \Sigma S_{23} S_{31} T_{12} , \\
& \Sigma T_{23} T_{31} S_{12} , \Sigma S_{23}^3 T_{23} , \Sigma T_{23}^3 S_{23} , \\
& \Sigma S_{11} T_{23}^2 , \Sigma S_{11}^2 T_{23}^2 , \Sigma T_{11} S_{23}^2 , \Sigma T_{11}^2 S_{23}^2 , \\
& \Sigma S_{11} S_{23} T_{23} , \Sigma S_{11}^2 S_{23} T_{23} , \Sigma T_{11} S_{23} T_{23} , \Sigma T_{11}^2 S_{23} T_{23} . \\
3. \quad & \Sigma S_{11} T_{23} U_{23} , \Sigma S_{11}^2 T_{23} U_{23} , \Sigma T_{11} S_{23} U_{23} , \Sigma T_{11}^2 S_{23} U_{23} , \\
& \Sigma U_{11} S_{23} T_{23} , \Sigma U_{11}^2 S_{23} T_{23} , \Sigma S_{23} (T_{31} U_{12} + T_{12} U_{31}) .
\end{aligned} \tag{4.2.24}$$



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