

REPRESENTATION THEORY

OF FINITE GROUPS

by

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To my parents and my husband, Christopher to whom I am eternally grateful for their encouragement and tolerance throughout this work.

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ABSTRACT

Three different types of group representations have been considered together with their possible applications. These are atom and bond representations which are topologically-relevant representations of the molecular symmetry group, projective representations which, although still composed of sets of unitary matrices, obey a modified group multiplication rule and corepresentations which consist of sets of matrices half of which are unitary and half anti-unitary.

Atom and bond representations are defined as reducible representations of a molecular point group which serve to describe the topological structure and composition of a molecule. They are amenable to computer storage and methods are given for resolving these representations into irreducible representations which correspond to equivalent sets of atoms or bonds. It is shown how bond representations can be derived from atom representations and a set of tables of both atom and bond representations is included. Application to additivity formulations of molecular properties is indicated, together with structural details of molecules and the identification of bending, stretching and redundant vibrational modes.

All different representation groups of the point groups are established and their character tables presented. These enable the construction of equivalent alternative sets of projective representations as well as to provide an easy route to the determination of double and space group representations. The construction of the representation group

clears up incompatibilities in already published literature on character systems for projective representations and shows that of all different methods available for the construction of these representations this one is most likely to be free from errors. The availability of alternative representation groups allows greater scope for the processes of ascent and descent in symmetry. Correlation tables are provided for the representation groups as well as tables of the symmetrized squares and cubes of projective representations.

The set of single and double valued corepresentations for each black and white magnetic group is identified with the vector representation of one or two abstract groups of known structure and character table. This facilitates the construction of the character tables (complete sets of which are presented for the first time) and reveals that in those cases where one abstract group is sufficient a formal character theory for providing symmetrized powers of corepresentations can be established, contrary to recent indications. Two types of cases are found where it is convenient to transform Wigner's corepresentation matrices and it is shown that normal group theoretical analysis can only be applied to Wigner's first type of corepresentation if his concept of physical equivalence is replaced by a group theoretical concept.

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CHAPTER 1

INTRODUCTION TO REPRESENTATION THEORY

1.1 HISTORICAL REVIEW

The first development of the concept of a "group" arose from the theory of algebraic equations. The problem was to find the solutions X_1, X_2, \dots, X_n to an algebraic equation of degree n ,

$$a_n X^n + a_{n-1} X^{n-1} \dots + a_1 X + a_0 = 0$$

with arbitrary coefficients, a_i . In 1771, Lagrange (1) discovered that these solutions for equations of degree two, three, or four were interpretable in terms of sets of permutations on two, three, or four elements which had the property that composition of two permutations belonging to the set resulted in a third permutation of the same set. He recognised that substitutions and permutations were a special case of linear substitutions and could be represented as a group of linear transformations or permutation matrices.

Cayley in 1878 (2), noted that abstract groups and hence all groups could be regarded as permutation groups. These ideas were further developed by Gauss in 1801 (3) and Abel in 1829 (4). The real importance of the group concept for the theory of algebraic equations was established by Galois in 1830 (5), who first used the term "group theory". Klein in 1876 (6) and Lie in 1893 (7) extended the group concept to other domains in mathematics. Instead of permutations, the group elements now acquired a more general meaning as transformations, or symmetry operations on geometric figures. The first general set of group postulates were given by Kronecker in 1870 (8).

The central figure in the history of group representation theory is Georg Frobenius who created the theory of group characters and much of representation theory. His first paper on the matrix representations of groups was presented at the November 18th, 1897 meeting of the Prussian Academy of Sciences at Berlin, where he was led to his discoveries by his analysis in 1896 of the group determinant. Dedekind (10) introduced this idea of group determinant and proposed its study to Frobenius. The problem concerning the group determinant was as follows:

Let G be a finite group with elements $g_1, g_2 \dots g_n$, where g_1 is equal to the identity. Associated with each element g_i is a variable $X_i = X_{g_i}$ where the polynomial Θ in $X_1 \dots X_n$ is defined by

$$\Theta(X_1 \dots X_n) = \begin{vmatrix} X_{g_1 g_1}^{-1} & X_{g_1 g_2}^{-1} & \dots & X_{g_1 g_n}^{-1} \\ X_{g_2 g_1}^{-1} & X_{g_2 g_2}^{-1} & \dots & X_{g_2 g_n}^{-1} \\ \dots & \dots & \dots & \dots \\ X_{g_n g_1}^{-1} & X_{g_n g_2}^{-1} & \dots & X_{g_n g_n}^{-1} \end{vmatrix}$$

and $X_{g_i g_j}^{-1}$ denotes X_k for k such that $g_i g_j^{-1} = g_k$.

Frobenius recognised that the decomposition of the group determinant into irreducible factors was equivalent to the decomposition of the regular representation into irreducible representations and that the degeneracies of the representations corresponded to the degrees of the factors in the group determinant. He also realized that matrix representations of groups were important from a practical point of view, since many groups have their natural representations in terms of matrices. Examples of these include the groups

which are isomorphic to groups of geometrical operations in three-dimensional space, or those representing groups of operations in quantum mechanics operating on the vectors of a Hilbert space.

Burnside, in his book of 1911 (11) rediscovered independently the chief results of Frobenius's early papers. However, he achieved his results from the theory of hyper-complex numbers which provided the link between the theories of finite and continuous groups; the link was made through the idea of the algebra of a finite group. This was based on the recognition of that special class of hyper-complex systems, the elements of which could be expressed in the form

$$\sum_{i,j=1}^n a_{ij} e_{ij}$$

where the n^2 basis elements e_{ij} can be multiplied according to the rule

$$e_{ij} e_{kl} = \delta_{jk} e_{il}$$

Reflecting upon the mathematics of the nineteenth century, J. Pierpoint wrote in 1904 (12)

"The group concept, hardly noticeable at the beginning of the century, has, at its close, become one of the fundamental and most fruitful notions in the whole range of our science".

1.2. WHAT IS A REPRESENTATION?

A representation of an abstract group, G , is a homomorphism ϕ of G onto a group T of non-singular linear operators acting on a finite-dimensional vector space, V , in a complex

field. Let $\phi g = T_g$ for all elements g of G . Then when ϕ is a representation

$$T_{g_1}(T_{g_2} X) = T_{g_1 g_2} X \quad \forall g_1, g_2 \in G \text{ and } \forall X \in V$$

An identity operator, T_E is defined such that

$$T_E X = X \quad \forall X \in V$$

Also $T_g^{-1} X = T_{g^{-1}} X \quad \forall g \in G \quad \text{and } \forall X \in V$

If the mapping $\phi : G \longrightarrow T$ conserves the multiplication laws of a group i.e.

$$\phi(g_1) \phi(g_2) = \phi(g_1 g_2)$$

for any pair of elements g_1, g_2 in G , then it is a homomorphism. If ϕ is an isomorphism the matrix images of G are called the faithful representations of G . Choosing a basis function $\langle X |$ consisting of linearly independent vectors X_1, X_2, \dots, X_d spanning the space V , matrices

$\Gamma_X(g)$ can be defined such that

$$T_g X_i = \sum_{j=1}^d X_j \Gamma_X(g)_{ij} \quad (i = 1, 2, \dots, d)$$

$\Gamma_X(g)$ is said to be the matrix representing g with respect to the basis $\langle X |$ in the representation ϕ . The set of all distinct matrices $\Gamma_X(g)$ is a matrix group and is the homomorphic image of G under the mapping $g \longrightarrow \Gamma_X(g)$. The kernel of the homomorphism is those elements of G which are mapped onto the unit matrix.

If $\langle X |$ and $\langle Y |$ are two bases of V defined such that

$$Y_k = \sum_{i=1}^d X_i S_{ik} \quad (k = 1 \text{ to } d)$$

and S is a non-singular matrix then

$$\Gamma_Y(g) = S^{-1} \Gamma_X(g) S$$

for all elements g of G . That is to say a change of basis leads to the matrix group $\Gamma_x(g)$ and $\Gamma_y(g)$ which are equivalent. It is always possible to choose a basis $\langle z |$ in V such that $\Gamma_z(G)$ is a unitary matrix group obeying the relationship

$$\Gamma(g^{-1})_{ij} = \Gamma^*(g)_{ji}$$

where the asterisk denotes complex conjugation.

If ϕ is a representation of G such that $T = \phi G$ is a group of non-singular linear operators acting in a vector space, V , then U will be an invariant subspace of V under T if U is a vector subspace of V and

$$Tg X \in U \text{ for all } Tg \in T \text{ and all } X \in U$$

If V has no proper invariant subspace under T then ϕ is an irreducible representation. If V can be split up into the direct sum of subspaces, each of which is invariant under T and each of which is the carrier space for an irreducible representation of G , then ϕ is said to be completely reducible.

An important result in representation theory is obtained from Schur's lemma which states:

"If $\Gamma(g)$ and $\Gamma'(g)$ are two irreducible representations of G such that

$$\Gamma(g) S = S \Gamma'(g) \text{ for all elements } g \text{ of } G$$
 then either S equals zero or is a non-singular matrix and $\Gamma(g)$ is equivalent to $\Gamma'(g)$ ".

A consequence of this is the fact that a representation is irreducible if and only if, the only matrices which commute with all matrices of the representation are scalar multiples of the unit matrix. In addition $\Gamma(g)$ is an irreducible representation if and only if

$$\frac{1}{|G|} \sum_{i=1}^{|G|} \left| \chi_{\phi}(g_i) \right|^2 = 1$$

where $|G|$ is the order of G and $\chi_{\phi}(g_i)$ is the character of $\Gamma(g_i)$ i.e. the trace or the spur of the matrix.

Other essential theorems about group representations include

1. The number of representations of a group is equal to the number of conjugacy classes, r , where each conjugacy class consists of the set of elements of the type $X^{-1}gX$ where X runs through all the elements of the group, G .
2. The sum of the squares of the degeneracies of the irreducible representations of G is equal to the order of G .
3. Two irreducible representations are orthogonal if

$$\sum_{j=1}^{|G|} \Gamma^{i*}(g_j)_{pv} \Gamma^k(g_j)_{qw} = \frac{|G|}{d_i} \delta^{ik} \delta_{pq} \delta_{vw}$$

where $\Gamma^i(g_j)_{pq}$ is the (pq) -th element of the matrix representative of g_j in the representation Γ^i with d_i equal to the dimension of Γ^i . Also

$$\begin{aligned} \delta^{ik} &= 1 \text{ if } \Gamma^i \text{ is identical to } \Gamma^k \\ &= 0 \text{ if } \Gamma^i \text{ is not equivalent to } \Gamma^k \end{aligned}$$

4. The matrix representatives reproduce the group multiplication table of elements of G .

1.3 EXTENSION OF THE CONCEPT OF A REPRESENTATION OF A FINITE GROUP

Ordinary or vector representatives as discussed in the

previous section have important applications in numerous physical problems, as will be seen in following sections. However, the concept of a representation can be extended in several different ways to deal with physical properties that so far representation theory has not been able to explain.

One of these problems is the inclusion of the effects of electron spin into the molecular or crystal system. Vector representations correspond to the single-valued representations of the spherical rotation group and describe systems that have zero or integral spin. However, if the total angular momentum, J , has half-integral values (i.e. the ions have an odd number of electrons) the required representations of the rotation group must be double-valued. This means that the quantum number, j , forms a basis for the character of the representation under a given symmetry operation, if j is an integer, the character of the rotations through an angle α is given by

$$\chi(\alpha) = \frac{\sin(j + \frac{1}{2})\alpha}{\sin \frac{1}{2}\alpha}$$

$$\text{and } \chi(\alpha) = \chi(\alpha + 2\pi)$$

therefore 2π is the identity operator. For half-integral values of j ,

$$\chi(\alpha + 2\pi) = -\chi(\alpha)$$

$$\chi(\alpha + 4\pi) = \chi(\alpha)$$

hence 4π is now the identity operation. This leads to the concept of the double group, which was in fact introduced by Frobenius (13) calling these groups binary groups and producing character tables for them. Bethe (14) realized the application of double groups to systems of ions with an

odd number of electrons, and calculation of these double-valued representations was given by Opechowski (15).

Other types of representations that are of use in physical problems are the so-called "representations up to a factor" or projective or ray representations. The concept of projective representation was introduced by Schur (16,17). They play an important role in the theory of non-symmorphic space groups, and are quite generally of importance for many quantum-mechanical systems because quantum-mechanical states are described by rays rather than by vectors of a Hilbert space. Such systems are systems of particles with half integral spin (i.e. in connection with the double groups previously mentioned) and those of charged particles in an electromagnetic field (in connection with gauge transformations).

If one non-singular n by n matrix $D(g)$ is assigned to each element g of a group G such that

$$D(g_1) D(g_2) = \omega(g_1, g_2) D(g_1 g_2)$$

(where $\omega(g_1, g_2)$ is a complex number) for all g_1 and g_2 in G , then the set of matrices $D(g_1), D(g_2) \dots$ is called an n th degree projective representation of G and the constants $\omega(g_1, g_2)$ is called the factor system. The projective representations of a finite abstract group, G , can be found by a mapping process from a covering group of G called the representation group.

When dealing with crystal systems that have magnetic properties, a new type of group must be introduced whose representations are called corepresentations. Normally, the symmetry elements of the group leave the time averaged atomic positions and electronic charge density invariant.

However, if the crystal possesses unpaired electrons it is possible for the equilibrium state to have a nonvanishing time averaged magnetic moment density as with ferromagnetic, antiferromagnetic, and ferrimagnetic crystals. Shubnikov (18) introduced the idea of antisymmetry by introducing an extra co-ordinate into the crystal system which is only allowed to take one of two values to deal with these magnetic structures. These new series of groups are called the black and white magnetic groups where the operation of antisymmetry occurs in half of the elements of the group. The other type of magnetic groups are the grey groups where the operation of antisymmetry is itself an element of the group and describes paramagnetic or diamagnetic crystals where the time averaged magnetic moment is zero.

In fact this operation of antisymmetry is the operation of time inversion, Θ , and as shown by Wigner (19) is an anti-unitary, antilinear operator, since the effect of Θ on the wave function is to change it into its complex conjugate. All representative matrices so far discussed have been unitary obeying the condition

$$D(g) D(\tilde{g}^*) = 1 \quad \text{for all elements } g \text{ of } G$$

However, in this case due to the fact that half of the symmetry elements of the magnetic group are antiunitary, this leads to a new set of multiplication rules for their corepresentations. If u is a unitary operator and a an antiunitary operator of G then

$$D(u_i) D(u_j) = D(u_i u_j)$$

$$D(u) D(a) = D(u a)$$

$$D(a) D^*(u) = D(a u)$$

$$D(a_i) D^*(a_j) = D(a_i a_j)$$

where the asterisks denote complex conjugation.

It can now be seen that a special type of algebra has been introduced to deal with the various types of representations of finite group mentioned above. However, this restricts the mathematics of representations to the extent that a lot of manipulations and theory used when dealing with vector representations is no longer applicable. One of the main results of the following work is the recognition of these special types of representations as ordinary representations of finite abstract groups. Since when the restrictions on these representations have been lifted it is possible to formulate a fuller and more accurate account of the physical properties described by these irreducible representations. Chapters 3, 4 and 5 deal with the study of projective representations and their application to double groups and space groups. Chapter 6 deals with the theory and applications of corepresentations in magnetic systems. As will be seen, this approach also clears up demonstrable errors in previously published mutually incompatible results between various sets of projective representations and leads to much simpler calculations when dealing with either projective representations or corepresentations. The creation of the representation groups needed to find the projective representations of the point groups also produces more abstract group tables than are readily available.

1.4 SOME APPLICATIONS OF REPRESENTATION THEORY TO CHEMICAL AND PHYSICAL PROBLEMS

The foundations of the application of group theory

(more precisely representation theory) in quantum mechanics were laid around 1930 principally by Weyl (20) and Wigner (21,22). From early work on crystal-field theory by Bethe (14) and on electronic band structures by Bouckaert, Smoluchowski and Wigner (23) it became apparent that the key to much of the exploitation of symmetry in the quantum mechanics of a molecule or solid lay in the irreducible representations of the classical point groups and space groups.

One of the basic chemical problems is always the determination of the structure of a molecule or crystal i.e. how atoms in a molecule are related to each other in space, and how these individual molecules are related to one another in a crystal lattice. The first part of the following work deals with these atom and bond representations. Atom and bond representations of a molecule are defined such that they are the reducible representations of the molecular point group spanned by the sets of atoms or bonds in the molecule.

One of the fundamental theories to group theoretical applications was enunciated by Wigner (21). He showed that for a system belonging to an abstract group G , any wave function $\Psi(r)$ of the system must belong to, i.e. must transform according to, one or other of the irreducible representations Γ^i of G . That is to say the wave function of a particle or quasi-particle in a molecule or crystal must be one component of a basis of one of the irreducible representations of G of that molecule or crystal. The degeneracies of energy levels can be predicted since they are determined by the degeneracies of the irreducible representations of G . Wigner applied this theorem to the classification of the normal modes of a vibrating system, and showed how any normal

mode transformed according to one or other of the irreducible representations of the group of the symmetry operations of that molecule. Also exactly how many normal modes there are belonging to each of the irreducible representations of the group and to find the exact form of each of the normal modes i.e. to find the normal co-ordinates.

Considering the electron in a hydrogen atom the potential in which it moves is just the potential due to the nucleus which is equivalent to a point charge. The system as seen by the electron then has spherical symmetry and therefore the electronic wave function must transform according to one of the irreducible representations of the three-dimensional rotation group. This means that its wave function must be a basis of $D^{\ell}(\alpha\beta\gamma)$ where α, β, γ are the Euler angles of some rotation. When considering atoms more complicated than hydrogen various approximations are involved. For example, the wave function of the whole system is assumed to be able to be expressed as a product of the individual particle wave functions or rather as a properly antisymmetrized sum of products of individual wave functions. The potential field seen by any one of these electrons is assumed to be a radially-symmetric field due to the nucleus and all the other electrons, which is only an approximation. If the above approximations are accepted then the individual particle wave functions will transform according to the irreducible representations $D^{\ell}\{\alpha, \beta, \gamma\}$. The application of atom and bond representations to the problem of the normal modes of a vibrating system is discussed in chapter 2.

Again using Wigner's theorem, Bethe (14) applied it in solid state physics in connection with the splitting of

the atomic energy levels in crystalline solids. The eigenvalues and eigenfunctions of an electron must belong to the irreducible representations of the symmetry operations of the Hamiltonian, H , of the system containing the electrons. It is accepted that the wave function is not "a physically observable property" of a system although it can be used in the determination of the matrix elements which can then be related to various physical properties of the system, where the point group symmetry of the system will impose some restrictions on the allowed forms of the wave function. The Hamiltonian operator can be regarded as having the symmetry of the crystallographic point group or space group. In a similar way as when dealing with the normal modes of a vibrating system, in the case of a free atom the appropriate group is the three-dimensional rotation group. If an atom is part of a crystal structure the electrostatic potential which is experienced by an electron in that atom will no longer be spherically symmetrical but will have the symmetry of one of the crystallographic point groups G . This often results in the partial or complete lifting of the degeneracy of the states of a given angular momentum quantum number. All quantum numbers with the exception of the so-called principal quantum number are indices characterizing irreducible representations of groups. Group theory can, if the symmetry of the crystal is known, give a qualitative description of the splitting.

This was extended, to include the effects of electron spin, into the double groups by Opechowski (15). The wave function of a system of identical particles is either symmetric or antisymmetric to the interchange of two identical

particles. For Bosons, having integral or zero spin, the wave function is symmetric and so is related to the single-valued representations of the molecular or crystal point group or space group. However, for Fermions, having half-integral values of spin, the wave function is antisymmetric and belongs to the double-valued representations of the molecular or crystal point group or space group.

A useful application to the study of molecules was made by Jahn and Teller (24) and Jahn (25). They found that by considering only the orbital part of the wave function, then with the sole exception of linear molecules, if the electronic wave function belongs to one of the degenerate representations of the molecular point group, the molecule is liable to instability due to vibrational interaction.

Similarly, when considering selection rules in the molecule or crystal system, if the wave functions Ψ_i of the individual atoms or molecules belong to the irreducible representations of the appropriate abstract group, under a physical influence, represented by the quantum-mechanical operator, P , a transition between states i and j is forbidden if the transition probability is zero i.e.

$$\int \Psi_j^* P \Psi_i d\tau = 0$$

$\int \Psi_j^* P \Psi_i d\tau$ is a physical observable and hence belongs to the totally symmetric representation of the group. Group theory can find the condition that has to be satisfied by two states i and j between which transitions are to be investigated. For an allowed transition, $\Psi_j^* P \Psi_i$ must belong to the totally symmetric, A_1 , representation of the group. This can be written as $\Psi_j^* (P \Psi_i)$ hence the direct product of the

two representations to which Ψ_j^* and $P\Psi_i$ belong must contain A_1 . Ψ_j^* belongs to an irreducible representation but $(P\Psi_i)$ may be reducible. Therefore, the direct product representation of $P\Psi_i$ must contain the representation to which Ψ_j^* belongs if the matrix element is to be non zero.

In summary, group representations are important when dealing with problems in valence theory and molecular dynamics, the description of the symmetry of crystals, and is of fundamental importance in quantum physics where it reveals the essential features which are independent of any special form of the dynamical laws and of any special assumptions concerning the forces involved. Among these numerous uses of representations are the labelling and degeneracy of electronic energy bands, the description of one or many electron wave functions, calculation of crystal field splitting, magnetic ordering in crystals where the operation of time-inversion is considered, labelling and degeneracy of dispersion curves for phonons, magnons and other quasi-particle states in a crystal, structure determination and application to phase transitions. A comprehensive study of recent developments in the use of group theory in solid state physics has been given in a review by Cracknell (26).

CHAPTER 2

THEORY AND APPLICATION OF ATOM AND BOND REPRESENTATIONS

2.1 INTRODUCTION

The understanding of molecular structure has always been one of the basic problems of chemistry; we need to know how atoms in a molecule are related to each other in space and how these individual molecules are related to one another in a crystal i.e. the symmetry properties of the molecule or crystal. One of the uses of symmetry considerations is the recognition of equivalent atoms in a molecule which will, for example, show that there is only one possible monsubstituted ethane but two possible monsubstituted propanes. Symmetry considerations alone can give a complete and rigorous answer to the question "what is possible and what is completely impossible". For example from symmetry considerations, the number of vibrational modes, their activity in the infra-red and Raman can be deduced.

These fundamental ideas lead to the theory of atom and bond representations. The atom or bond representation of a molecule is that reducible representation of the molecular point group spanned by the set of atoms, or bonds in the molecule. The topological structure of a molecule is defined by its atom and bond representations, and since they are group representations, they permit a fuller description of a molecule than is possible with graph theory. It will be seen that these atom and bond representations are particularly amenable to computer storage of this data which describes the molecule's symmetry. Methods will be intro-

duced which enable the resolution of these atom and bond representations into irreducible representations corresponding to equivalent sets of atoms or bonds; the bond representations being deducible from the atom representations. They have an application to additivity properties of molecules and also in the prediction of bending, stretching and redundant vibrational modes.

2.2 THEORY OF ATOM REPRESENTATIONS

In the same way that the set of atoms in a molecule can be resolved into subsets of equivalent atoms, the atom representation of a molecule can be regarded as built up from the atom representations of the subsets of equivalent atoms. The atom representation of a subset of m equivalent atoms occupying sites of symmetry group H (order h) in a molecule of symmetry group G (order g) is that $n (=g/h)$ - dimensional reducible representation of G obtained by ascent in symmetry (Boyle, 27) from the totally symmetric representation of H . Thus for the hydrogen atoms in methane, $G = T_d$, $H = C_{3v}$ and hence from Table 5 of Boyle the H_4 -atom representation is A_1+T_2 . This is four-dimensional since there are four ($= 24/6$) atoms and contains the totally symmetric, A_1 , representation of G once since the four atoms belong to a single subset of equivalent atoms. The atom representation of the carbon atom in methane is A_1 since $H=G$. The atom representation of methane is therefore $2A_1+T_2$. The utility of storing this information as $2A_1+T_2$ rather than $(A_1)_c + (A_1+T_2)_H$ is only assured if atom representations can be resolved uniquely into the atom representations of the sub-

sets of equivalent atoms. It will be shown that this can always be done, although it involves the rather novel step for representation theory of resolving a reducible representation into \dagger reducible representations. Such resolutions will not only be required to regenerate the input information but also to resolve the problem of identifying the different subsets of equivalent atoms obtained from certain distortions of a molecule. Thus if the methane molecule is distorted along a three-fold axis so that $G' \cong C_{3v}$ then the H-atom representation is obtained by descent in symmetry from G to G' as $2A_1+E$. This is in fact the sum of A_1 and A_1+E , i.e. atom representations of different subsets of equivalent atoms in the distorted molecule.

There are only five different kinds of site symmetry in tetrahedral molecules and hence all atom representations can be built up from just five reducible representations corresponding to the different types of site symmetry. These are enumerated in table 1

Site Symmetry	Atom Representation	Number of Equivalent Atoms	Number of Equivalent Sets of Atoms	Symmetry of Point Complex
T_d	A_1	1	m_0	K_h
C_{3v}	A_1+T_2	4	m_3	T_d
C_{2v}	A_1+E+T_2	6	m_2	O_h
C_{1h}	$A_1+E+T_1+2T_2$	12	m_d	T_d
C_1	$A_1+A_2+2E+3T_1+3T_2$	24	m	T_d

Table 1. The atom representations of sets of equivalent atoms in tetrahedral molecules.

In the fourth column of Table 1, the number of sets of atoms of a given site symmetry is denoted by the traditional notation used in connection with Brester's tables for analyzing molecular vibrations. This enables the total number of atoms, N , of the molecule to be expressed as

$$N = m_0 + 4m_3 + 6m_2 + 12m_d + 24m$$

If the constituent atom representations are denoted as $D(m_0)$, $D(m_3)$ etc, the total atom representation D^A , may be written

$$D^A = m_0 D(m_0) + m_3 D(m_3) + m_2 D(m_2) + m_d D(m_d) + m D(m)$$

and also

$$D^A = f(A_1)A_1 + f(A_2)A_2 + f(E)E + f(T_1)T_1 + f(T_2)T_2$$

where the f 's are frequency factors specifying the occurrence of the irreducible representations of T_d in the atom representation D^A . These frequency factors are entirely determined by the number of site symmetries as

$$f(A_1) = m_0 + m_3 + m_2 + m_d + m$$

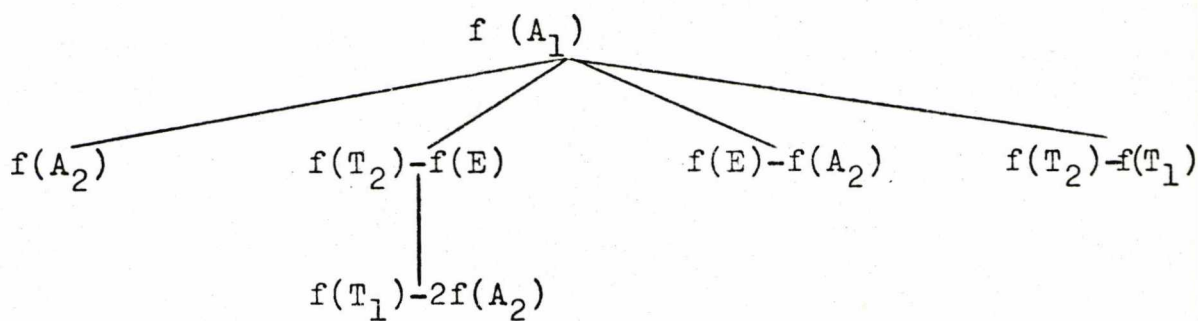
$$f(A_2) = m$$

$$f(E) = m_2 + m_d + 2m$$

$$f(T_1) = m_d + 3m$$

$$f(T_2) = m_3 + m_2 + 2m_d + 3m$$

However, each of the five m 's cannot be negative and hence five inequalities exist which govern the relative magnitude of the frequency factors. These can be illustrated in the following diagram in which each tie-line represents an inequality in the sense that the function above must be greater than or equal to the function below. Further each function is a non-negative integer.

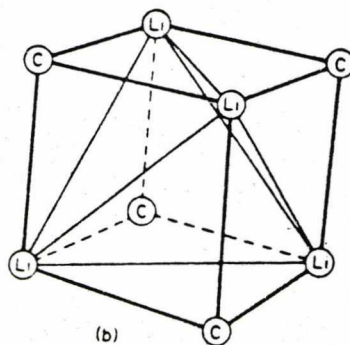
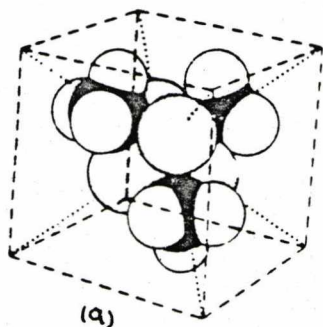


There is another inequality which is entirely physical in origin. The occupation number, m , of the central site can never be greater than one and hence

$$1 \geq f(A_1) - f(A_2) + f(T_1) - f(T_2) \geq 0$$

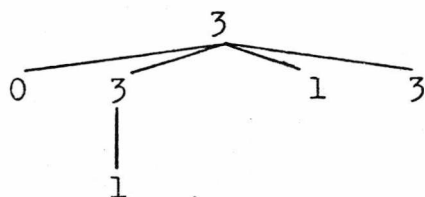
The restrictions on the frequency factors imply that not all possible reducible representations can be atom representations and the diagrams provide a simple method (which is very appropriate for transcription into a computer programme) for determining the acceptability of a reducible representation for the analysis which is to follow.

An illustration of this is in consideration of the molecule $(CH_3Li)_4$ shown below



The structure of $(\text{CH}_3\text{Li})_4$ is that suggested by Weiss and Lucker (28). Diagram (a) shows the tetrahedral Li_4 unit with the CH_3 groups located symmetrically above each face of the tetrahedron. Diagram (b) shows how the structure can also be regarded as derived from a cube.

The reducible representation $3A_1 + E + T_1 + 4T_2$ relevant to $(\text{CH}_3\text{Li})_4$ is now examined. Inserting the frequency factors into the diagram yields



which is acceptable. Further, the physical criterion $1 \gg 0 \gg 0$ is also satisfied.

Finally a criterion is needed to decide whether the molecule is actually tetrahedral, or whether it actually belongs to a higher symmetry group and is just being described by tetrahedral symmetry. The atom representation $D^A = 2A_1 + E + T_2 = D(m_0) + D(m_2)$ meets the preceding criteria but in fact describes an octahedral molecule of ML_6 type. The solution of this problem is to examine the symmetry of the "point complexes" as defined by Niggli (29). These are the symmetries of the equivalent sets taken in isolation and have been included in Table 1. Thus in the ML_6 complex, the isolated M atom has spherical (K_h) symmetry while the six L atoms form a point complex of octahedral (O_h) symmetry. The symmetry of the molecule is the intersection (due regard being paid to orientation, where relevant) of the symmetries of constituent point complexes. For a molecule to be tetra-

hedral at least one of the point complexes of site symmetry C_{3v} , C_{1h} , or C_1 must be occupied,

$$\text{i.e. } m_3 + m_d + m \gg 1$$

This could also be written as $f(T_2) - f(E) \gg 1$ and hence also as an additional tie-line in the diagram.

The resolution of atom representations into the reducible representations of Table 1 is effected by expressing the number of site symmetries in terms of the frequency factors. Then

$$\begin{aligned} D^A = & [f(A_1) - f(A_2) + f(T_1) - f(T_2)] D(m_0) + [2f(A_2) - f(E) - \\ & f(T_1) + f(T_2)] D(m_3) \\ & + [f(A_2) - f(E) - f(T_1)] D(m_2) + [f(T_1) - 3f(A_2)] D(m_d) + \\ & f(A_2) D(m) \end{aligned}$$

and hence for $(CH_3Li)_4$, $m_3 = 2$, $m_d = 1$, $m_0 = m_2 = m = 0$. Since $D(m_3)$ is four-dimensional and $D(m_d)$ is twelve-dimensional, both carbon and lithium atoms form tetrahedra of four atoms while the hydrogen atoms lie in the reflection planes. The relative orientation of the tetrahedra and the bonding remains to be determined by the bond representations.

The example of tetrahedral molecules so far considered has been fortuitous in that the number of possible site symmetries equalled the number of irreducible representations and also the frequency factors were mutually independent. This has made the analysis of the atom representations fairly straightforward. However, this is not generally the case since there are the two further possibilities to consider, where in the first case the number of irreducible representations of the molecular point group exceeds the number of site symmetries and secondly where the number of irreducible

representations is less than the number of site symmetries.

The first case to be considered is the case for octahedral molecules, O_h , where the number of frequency factors exceeds the number of site symmetries on which they depend i.e. O_h has ten irreducible representations and only seven atomic site symmetries. This leads to some equalities that must be satisfied by the frequency factors. As for the tetrahedron the total number of atoms, N , of the molecule may be expressed as

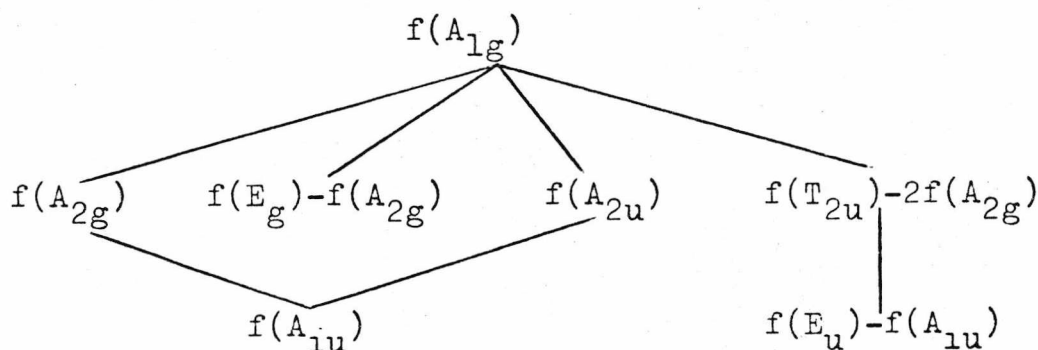
$$N = m_o + 6m_4 + 8m_3 + 12 m_{2v} + 24m_h + 24m_d + 48m$$

Hence for a reducible representation to be an atom representation of O_h the following three equalities and seven inequalities on the frequency factors must be satisfied

$$f(T_{1u}) = f(A_{2u}) + f(E_g)$$

$$f(T_{1g}) = f(A_{2g}) + f(E_u)$$

$$f(T_{2g}) = f(A_{2u}) - f(A_{2g}) + f(T_{2u})$$



There remains two inequalities to be satisfied, one which is the condition that there is only one or no atom at the centre of the octahedra and secondly the condition on the site symmetries for the molecule to have octahedral symmetry. These are

$$1 \gg f(A_{1g}) - f(E_g) - f(A_{1u}) + f(A_{2g}) + f(E_u) \gg 0$$

$$m_4 + m_3 + m_{2v} + m_h + m_d + m \gg 1$$

The opposite case to that of the octahedral example is for those cases where the number of irreducible representations is less than the number of site symmetries as is the case for those molecules with purely rotational symmetry of types D_n , T, O and I. The number of site symmetries exceed the number of frequency factors and hence the correct number of linearly-independent inequalities is composed of inequalities between the frequency factors and also restrictions on their absolute values. In such cases it is usually sufficient to include the condition $m \gg 1$ which guarantees their symmetry (Jahn and Teller, 30) in the construction of the inequality diagram.

Considering molecules possessing D_3 symmetry the simultaneous equations expressing the dependence of the frequency factors on the site symmetries are only solvable if the physical condition $0 \leq m_0 \leq 1$ is also included. The analysis proceeds as follows. There are four different sets of site symmetry in D_3 molecules shown in the following table

Site Symmetry	Atom Representation	Number of Equivalent Atoms	Number of Equivalent Sets of Atoms	Symmetry of Point Complex
D_3	A_1	1	$0 \leq m_0 \leq 1$	K_h
C_3	$A_1 + A_2$	2	$0 \leq m_3$	$D_{\infty h}$
C_2	$A_1 + E$	3	$0 \leq m_2$	D_{3h}
C_1	$A_1 + A_2 + 2E$	6	$1 \leq m$	D_3

The total number of atoms, N, of the molecule is

$$N = m_0 + 2m_3 + 3m_2 + 6m$$

The frequency factors can be expressed

$$f(A_1) = m_0 + m_3 + m_2 + m$$

$$f(A_2) = m_3 + m$$

$$f(E) = m_2 + 2m$$

Since the number of site symmetries is greater than the number of frequency factors this has to be resolved on a parity argument. From the above table it is seen that

$$f(A_1) - f(A_2) = m_0 + m_2$$

$$f(E) - 2f(A_2) = m_2 - 2m_3$$

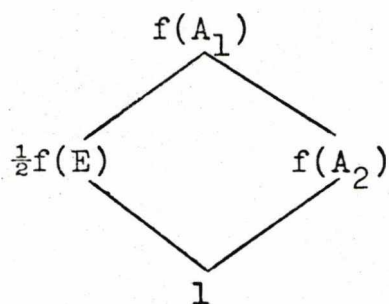
Consideration of the parity of these equations gives the following

m_2	m_0	$f(A_1) - f(A_2)$	$f(E) - 2f(A_2)$
odd	0	odd	odd
even	0	even	even
odd	1	even	odd
even	1	odd	even

Hence m_0 may be determined by $|f(A_1) + f(A_2) - f(E)| \bmod 2$, and now D^A may be uniquely resolved as

$$D^A = [|f(A_1) + f(A_2) - f(E)| \bmod 2] D(m_0) + \frac{1}{2} [f(A_1) + f(A_2) - f(E) - |f(A_1) + f(A_2) - f(E)| \bmod 2] D(m_3) + [f(A_1) - f(A_2) - |f(A_1) + f(A_2) - f(E)| \bmod 2] D(m_2) + \frac{1}{2} [f(A_2) - f(A_1) + f(E) + |f(A_1) + f(A_2) - f(E)| \bmod 2] D(m)$$

The atom representations must obey the equality



The normal process of descent in symmetry can be applied to atom representations and by examining the acceptability of atom representations derived in this way one can decide which symmetries are obtainable by distortion. Thus descent in symmetry from the atom representation $2A_{1g} + E_g + T_{1u}$ of O_h to D_3 yields the acceptable atom representation $2A_1 + A_2 + 2E$ and hence ML_6 molecules can be distorted to a D_3 structure. However, boron trifluoride, BF_3 , which has the atom representation $2A'_1 + E'$ of D_{3h} cannot be distorted to D_3 symmetry since $2A_1 + E$ is not an acceptable atom representation of D_3 . Descent in symmetry between atom representations can also be used to determine whether any sets of equivalent atoms have split into two or more such sets on distortion. The number of equivalent sets (or point complexes) occupied is the number of totally symmetric representations contained in the atom representation. Thus distortion of ML_6 from O_h to D_3 symmetry does not cause any splitting of sets of equivalent atoms since the atom representation contains the same number of totally symmetric representations in both symmetries.

2.3 THEORY OF BOND REPRESENTATIONS

For some purposes, the atom representation of a molecule will be a sufficient means of classifying its

structure. However, in general it is helpful to be able to specify which pair of atoms are connected by bonds. The site symmetry of a bond may be defined as those elements of the molecular point group which leave the bond in situ: in the case of homopolar bonds (i.e. those between equivalent atoms) those symmetry operations which interchange the ends of the bond are also included. In all cases the bond site symmetry is the symmetry of the mid-point of the bond, though it is only in the case of homopolar bonds that this is a special point. Bond representations can thus be generated by ascent in symmetry from the totally symmetric representation of the symmetry group of the mid-point. The bond representation of a molecule can be defined as the sum of the bond representations corresponding to the equivalent sets of bonds within the molecule. Thus the octahedral ML_6 molecule would have different bond representations according to whether the M-L bonding was supplemented by L-L bonding or not.

Atom and bond representations can be related group theoretically by the following argument. An atomic property, P^A , of a molecule can be written as a sum of one-atom functions, f_i

$$\text{i.e. } P^A = \sum_{\substack{\text{all atoms} \\ i}} f_i$$

whereas a bond property, P^B , is a sum of two-atom functions, g_{ij}

$$P^B = \sum_{i > j} g_{ij}$$

In the case of bonds between different equivalent sets of atoms, the atoms can be numbered so that $i > j$ where i runs

over one set and j the other. By writing

$$g_{ij} = f_i' f_j''$$

$$\text{Then } P^B = \sum_{i > j} g_{ij} = \sum_i f_i' \sum_j f_j'' = (P^A)' (P^A)''$$

Now the symmetry of the atom representations of the two sets is not necessarily the same and hence the symmetry of the bond representation, D^B is

$$D^B = (D^A)' (D^A)''$$

i.e. the direct product of the atom representations of the two sets of atoms involved.

In the case of bonds within a single equivalent set of atoms, the dummy indices i and j run over the same range and the bond function g_{ij} must be of the type

$$g_{ij} = f_i' f_j'' + f_j' f_i''$$

An atom function can be defined on the basis of

$$f_i = f_i' f_i''$$

Then

$$\begin{aligned} P^B &= \sum_{i > j} g_{ij} = \sum_{i > j} (f_i' f_j'' + f_j' f_i'') \\ &= \sum_i f_i' \sum_j f_j'' - \sum_i f_i' f_i'' \\ &= (P^A)' (P^A)'' - P^A \end{aligned}$$

Now the symmetry of $(P^A)'$ and $(P^A)''$ must be identical and the symmetry of $(P^A)' (P^A)''$ must be symmetric to interchange of primes and hence is the symmetry of the symmetric square, $[(D^A)^2]$ of the atom representation, D^A .

Hence

$$D^B = [(D^A)^2] - D^A$$

for bonds between equivalent atoms.

The bond representations generated by these formulae for D^B will certainly include all possible chemical bonds between the atoms considered. Chemically, however, bonds are not recognized if they would have to intersect other bonds e.g. trans - (L,L) bonds in ML_6 complexes are disallowed, quite independently of recognizing M-L bonding instead. The midpoint of every chemical bond is a possible atomic site hence the bond representation of a set of equivalent bonds is always isomorphic with an atom representation. The bond representations for the tetrahedral P_4 molecule is isomorphic with the atom representation $A_1 + E + T_2$ and is not restricted by the fact that this representation would not be acceptable as an atom representation. Although D^B is subject to different acceptability criteria, the analysis of an acceptable D^B can be performed with the same formulae as for an atom representation. This is because the chemically-allowed bond representations of equivalent sets of bonds are isomorphic to those atom representations which correspond to atomic site symmetries which are also subgroups of $D_{\infty h}$, the symmetry of an isolated bond. The chemically forbidden bond representations are those for which the apparent site symmetry (i.e. that of the midpoint) is a subgroup of the molecular point group which, due regard being paid to the orientation of symmetry elements, is either not allowed as an atomic site symmetry and/or the point of intersection of the bonds corresponds to a point which actually has a higher symmetry than that of the midpoint of the bonds.

Resolution processes are needed for bond representations which have been obtained from atom representations by the processes described above and also for bond representations which are constructed from a known molecular structure for storage in a computer. The latter problem presents no additional difficulties as all chemical bond representations will be isomorphic with atom representations for which a resolution process has been devised in the preceding section. The former problem, however, requires the recognition and elimination of those chemically forbidden bond representations which are not isomorphic with atom representations. Such difficulties only arise when dealing with the bonds within a single equivalent set of atoms as all non-chemical bonds between inequivalent sets, even those of the same symmetry, have apparent site symmetries which are possible atomic site symmetries. To illustrate the problem, the sets of all possible bonds within given equivalent sets of atoms of a tetrahedral molecule can be resolved as follows:

		<u>Apparent Site Symmetries</u>	
D^A	$[(D^A)^2] - D^A$	Chemical Bonds	Non-chemical Bonds
$D(m_3)$	$A_1 + E + T_2$	C_{2v}	—
$D(m_2)$	$2A_1 + 2E + T_1 + 2T_2$	C_{1h}	D_{2d}
$D(m_h)$	$5A_1 + 2A_2 + 7E + 6T_1 + 9T_2$	$C_{2v}, 2C_{1h}$	C_2, C_1
$D(m)$	$16A_1 + 10A_2 + 26E + 30T_1 + 36T_2$	$5C_{1h}, 2C_1$	$3C_2, C_{1h}, 5C_1$

Table 2. Resolution of the sets of bonds within given equivalent sets of atoms in tetrahedral molecules.

It can be seen from Table 2 that the only apparent site

symmetries not occurring as atomic site symmetries are D_{2d} and C_2 and the table indicates when they need to be eliminated from the expression $[(D^A)^2] - D^A$ before this can be resolved into sets of equivalent bonds using the formula for atom representations. Similar analysis can be presented for all other point symmetries. In the case of the $(CH_3Li)_4$ molecule, the C-Li bonds must be contained in the representation

$$\begin{aligned} (D^A)_C \times (D^A)_{Li} &= D(m_3) \times D(m_3) = (A_1+T_2)(A_1+T_2) = 2A_1+E+T_1+3T_2 \\ &= D(m_3) + D(m_d) \end{aligned}$$

Now if both carbon and lithium tetrahedra are positive, the $D(m_3)$ set is chemical and the $D(m_d)$ non-chemical, while if one tetrahedron is positive and the other negative, the reverse is true. In fact the C-Li bond representation is $D(m_d)$ and hence this specifies the relative orientation of the carbon and lithium tetrahedra in this molecule - a fact which could not have been deduced from the atom representation alone.

A full set of tables are included at the end of the chapter of the atom and bond representations for the molecular point groups. These have been generalized into group families wherever appropriate. To simplify the compilation of these tables the summations over the dummy index, r , have been abbreviated so that $\sum_{r=1}^{r=n}$ becomes $\sum n$ etc. The tables include all possible sets of equivalent atomic site symmetries given in a molecular structure, their atom representations, the number of equivalent sets of atoms of a given site symmetry denoted in the traditional way used in connection with Brester's tables for analysing molecular vibrations. The symmetry of the point complex is also given together with

the physical condition that there is only one or zero atoms at the centre of a molecule, and the symmetry condition that certain atomic sites must be occupied to conserve the symmetry of the molecule. The bond representations between atoms of equivalent sets have been split into the chemically allowed bonds and the non-chemical bonds i.e. the crossing bonds that will be predicted by use of the bond representation formula given previously.

2.4 APPLICATION OF ATOM AND BOND REPRESENTATIONS

The first application is the storage of structural and topological information about molecules in the computer. Examples of how this might be achieved are given in Table 3.

Molecule	Atom Representations	Bond Representations
P_4	$A_1 + T_2 = D(m_3)_p$	$A_1 + E + T_2 = D(m_2)_{p-p}$
CH_4	$2A_1 + T_2 = D(m_o)_c + D(m_3)_H$	$A_1 + T_2 = D(m_3)_{c-h}$
$Ni(CO)_4$	$3A_1 + 2T_2 = D(m_o)_{Ni} + D(m_3)_c + D(m_3)_o$	$2A_1 + 2T_2 = D(m_3)_{Ni-c} + D(m_3)_{c-o}$
$(CH_3Li)_4$	$3A_1 + E + T_1 + 4T_2 = D(m_3)_c + D(m_3)_{Li} + D(m_d)_H$	$2A_1 + 2E + 2T_1 + 4T_2 = D(m_d)_{C-Li} + D(m_d)_{C-H}$

Table 3. The atom and bond representations of some tetrahedral molecules

The resolution of the atom and bond representations indicated above provides a means of constructing additivity schemes for those physical properties which can be adequately treated

by such an empirical approach. A diamagnetic molecule possesses no resultant magnetic moment and the magnetic susceptibility, χ , has a negative value. Henrichsen (31), when studying the magnetic susceptibilities of organic compounds, observed that it was possible to assign definite susceptibility values to individual atoms which allowed a very rough estimate of susceptibilities, in accordance with the principle of additivity. He expressed the susceptibility of a diamagnetic organic compound by the additive formula

$$\chi = \sum \chi_A$$

where χ_A are the susceptibilities of the individual atoms comprising the molecule. This can be re-expressed in terms of atom representations by associating a partial molar susceptibility with each part of the atom representation corresponding to a different equivalent set of atoms. Pascal (32) refined Henrichsen's scheme by introducing correction factors due to the structural characteristics i.e. the bonds of the given molecule and therefore obtained much more accurate values for susceptibilities. This serves as a practical method for analysing the structure of molecules, since every atom can be assigned a unique value for χ_A while the structural corrections i.e. double or triple bond, aromatic or aliphatic ring etc., were experimentally determined. The correction factors can again be re-expressed in terms of the bond representations. The use of atom and bond representations is particularly useful when dealing with the anisotropic components of physical property tensors. Since each equivalent set of atoms can be regarded as a "point complex"

of symmetry greater than or equal to that of the molecule, we shall not be concerned with any components of the individual atoms which are averaged out in the whole molecule. Further, if the anisotropic component under investigation is averaged out in the symmetry of a "point complex", then the contribution of that part of the atom representation is necessarily zero. Thus in the study of tris-bidentate octahedral complexes of D_3 symmetry the contributions to the optical activity in an additivity scheme should only come from atoms in general (C_1) positions since only their point complex symmetry is that of a point group admitting optical activity. The same can be said of the bond contributions.

Atom and bond representations are also useful for visualizing the normal modes of vibration. Every molecule, at all temperatures is continually executing vibrational motions i.e. motions in which its distances and internal angles change periodically without producing any net translation of the centre of mass of the molecule or importing any net angular momentum to the molecule. These internal vibrations are the result of the superposition of a number of motions known as the normal modes of vibration. Since an atom has three degrees of motional freedom i.e. displacement in the x,y or z direction without necessary displacement in all three, a molecule consisting of n atoms will therefore have $3n$ degrees of freedom. However, of these three degrees of freedom three are translations and three correspond to molecular rotations hence the number of vibratory motions in a molecule is $3n - 6$. Except in the case of a linear molecule where there are $3n - 5$ vibrational modes since rotation of nuclei about the molecular axis cannot occur

since all nuclei lie on the axis. When considering the appropriate class of molecules the number of in-plane modes is $2n - 3$ and the number of out-of-plane modes $n - 3$.

In non-cyclic molecules the symmetry of the stretching modes is the bond representation, since the stretching of a bond is a scalar, or symmetry-preserving motion. The bending modes can be derived from atom representations. A bending mode preserves the symmetry of all points on the bisector of the angle between the bonds involved and is therefore to be associated with the representation which atoms placed on these bisectors would have. Such an atom representation is easily derived from the calculation of the midpoint symmetry described in the previous section. However, such calculations need to be modified to take account of redundancies amongst the symmetry co-ordinates. If S non-coplanar bonds meet at an atom there will be $\frac{1}{2} S(S-1)$ bond angles. However, these bond angles are not all independent of each other since if there are n atoms in the molecule, there will be $S+1$ non-coplanar bonds meeting at an atom. The number of stretches is equal to the number of bonds, S , hence the total number of bonds will be $3n - 6 - S$ and the total number of independent angles $3(S+1) - 6 - S = 2S - 3$. The symmetry of these redundant modes has therefore to be subtracted from the atom representation corresponding to the midpoints before this can be used to specify the bending modes. When there is only one redundant mode, this will be totally symmetric. When there are more than one redundant modes, their symmetry corresponds in general to a sum of chemical and non-chemical bond representations.

In the case of SF_6 , the redundant modes are of symmetry

$A_{1g} + E_g$ in O_h , i.e. the non-chemical bond representation corresponding to an apparent site symmetry D_{4h} . This occurs because the redundant co-ordinates correspond to the sum of the angles in each of the three planes of four fluorine atoms (each of which is separately of symmetry D_{4h}) being 360 degrees. In ethane, C_2H_4 , the redundant co-ordinates are each totally symmetric in C_{2v} , the site symmetry of the carbon atoms and the redundant modes are hence of symmetry $A_g + B_{1u}$ (choosing the C=C axis to be the z axis) of D_{2h} .

To illustrate the technique the normal modes of SF_6 are enumerated, which will also serve as a model for any ML_6 -type octahedral complex. There will be 15 normal modes of which the six stretching modes are isomorphic with the bond representation, viz $A_{1g} + E_g + T_{1u}$ of O_h . The midpoint of two cis-fluorine atoms is of C_{2v} symmetry and the corresponding atom representation is $A_{1g} + E_g + T_{1u} + T_{2g} + T_{2u}$. Casting out the $A_{1g} + E_g$ redundant modes leaves $T_{1u} + T_{2g} + T_{2u}$ as the nine bending modes. The sum of the stretching and bending modes is $A_{1g} + E_g + 2T_{1u} + T_{2g} + T_{2u}$ in agreement with the symmetries derived by the method of ascent in symmetry (Boyle, 27) or other methods. The following table gives a selection of molecules belonging to various molecular point group symmetries illustrating the above description.

MOLECULE	SYMMETRY	BOND REPRESENTATION		ANGLE REPRESENTATION		REDUNDANT
		\equiv STRETCH		\equiv BEND		ANGLE REPRESENTATION
SF ₆	O _h	A _{1g} +E _g +T _{1u} =D(m ₄) _{S-F}		A _{1g} +E _g +T _{2g} +T _{1u} +T _{2u} =D(m _{2v}) _{FSF}		A _{1g} + E _g
C ₂ H ₄	D _{2h}	A _g +B _{1u} +B _{2u} +B _{3u} =D(m _{h^{xy}}) _{C-H} + A _g = D(m _o) _{C-C}		A _g +B _{1u} +B _{2u} +B _{3u} =D(m _{h^{xy}}) _{HCC} + A _g +B _{1u} = D(m _{2v^z}) _{HCH}		A _{1g} + B _{1u}
PtCl ₄	D _{4h}	A _{1g} +B _{1g} +E _u =D(m _{2u}) _{Pt-Cl}		A _{1g} +B _{2g} +E _u =D(m _{2d}) _{ClPtCl}		A _{1g}
NH ₃	C _{3v}	A ₁ +E = D(m _h) _{C_{3v}-Cl}		A ₁ +E = D(m _h) _{HNH}		-
CH ₄	T _d	A ₁ +T ₂ = D(m _{3v}) _{C-H}		A ₁ +E+T ₂ = D(m _{2v}) _{HCH}		A ₁
BF ₃	D _{3h}	A ₁ ' + E' = D(m _{2v}) _{B-F}		A ₁ ' + E' = D(m _{2v}) _{FBF}		A ₁ '
N ₂ F ₂	C _{2h}	A _g +B _u = D(m _h) _{N-F} + A _g = D(m _{2h}) _{N-N}		A _g +B _u = D(m _h) _{FNN}		-
CHCl ₃	C _{3v}	A ₁ +E = D(m _h) _{C-Cl} A ₁ = D(m _{3v}) _{C-H}		A ₁ +E = D(m _h) _{ClCCl} +A ₁ + E = D(m _h) _{HCCl}		A ₁

In conclusion it may be noted that this work arose from an attempt to derive new chemically-useful information from graph theory. It appeared in the course of that study that apart from the applications reviewed by Rouvray (33), the technique was far too limited in power to generate anything more than a re-formulation of a structure and some interesting empirical formulae. Storage of bonding information in an adjacency matrix is far less efficient than in atom and bond representations for molecules with about four or more atoms. Further the power of representation theory allows derivation of midpoint symmetries and also to specify vibrational symmetries: graph theory is peculiarly insensitive to the symmetry of a structure. Thus the graph-theoretical description of PF_5 is independent of whether it is a trigonal bipyramid, right pyramid or a square base or some other structure with the same topology.

Atom Site Symmetry	Atom Representations	Number of Equivalent Sets Of Atoms	Symmetry of Point Complex	Bond Site Symmetry	
				Chemical Bonds	Non-Chemical Bonds
C_{2n-I}	A	m_o	K_h		
C_I	$A + \sum_{r=1}^{n-1} E_r$	m	$D_{(2n-I)h}$	$C_I(n \neq I)$	$(n-2)C_I$

Atom Representations

$$N = m_o + (2n-I)m$$

Chemical Condition

$$I \gg f(A) - f(E) \gg 0$$

Equality

$$f(E_1) = f(E_2) \dots = f(E_{n-I})$$

Symmetry Condition

Combinations of any two (w.r.t. orientation) must appear

Inequality

$$\begin{array}{c} f(A) \\ | \\ f(E) \end{array}$$

ATOM AND BOND REPRESENTATIONS FOR C_{2n-I} MOLECULES

Atom Site Symmetry	Atom representations	Number of Equivalent Sets of Atoms	Symmetry of Point Complex	Bond Site Symmetry	
				Chemical Bonds	Non-Chemical Bonds
C_{2n}	A	m_o	K_h		
C_I	$A+B+\sum_{r=1}^{n-1} E_r$	m	$D_{\infty h} (n=I)$ $D_{nh} (n=I)$	$C_2 (n=I)$ $C_I (n \neq I)$	$C_2, (n-2)C_I$

Atom Representations

$$N = m_o + 2nm$$

Chemical Condition

$$I \gg f(A) - f(B) \gg 0$$

Equality

$$f(B) = f(E_I) \dots \dots \dots = f(E_{n-I})$$

Symmetry Condition

Combinations of any two (w.r.t. orientation) must appear

Inequalities

$$\begin{array}{c} f(A) \\ | \\ f(B) \end{array}$$

ATOM AND BOND REPRESENTATIONS FOR C_{2n} MOLECULES

Atom Site Symmetry	Atom Representations	Number of Equivalent Sets of Atoms	Symmetry of Point Complex	Bond Site Symmetry	
				Chemical Bonds	Non-Chemical Bonds
$C_{(4n-2)h}$	A_g	m_o	K_h		
$C_{(4n-2)}$	$A_g + A_u$	m_{4n-2}	$D_{\infty h}$	$C_{(4n-2)h}$	
C_{Ih}	$A_g + B_u + \sum_{n-1} E_{2rg} + E_{(2r-1)u}$	m_h	$D_{\infty h} (n \neq I)$	$C_{2h} (n \neq I)$	$(2n-3)C_{Ih}$
			$D_{(4n-2)h} (n \neq I)$	$C_{Ih} (n \neq I)$	$C_{2h} (n \neq I)$
C_I	$A_g + A_u + B_g + B_u + \sum_{2n-2} E_{rg} + E_{ru}$	m	$D_{(4n-2)h}$	C_{Ih}	$C_2, S_2,$
				$C_I (n \neq I)$	$(4n-5)C_I (n \neq I)$

Atom Representations

$$N = m_o + 2m_{4n-2} + (4n-2)m_h + (8n-4)m$$

Chemical Condition

$$I \gg f(A_g) - f(A_u) + f(B_g) - f(B_u) \gg 0$$

Equality

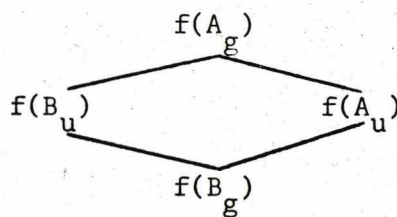
$$f(B_g) = f(E_{I_g}) = f(E_{2u}) \dots \dots \dots = f(E_{(2n-2)u})$$

$$f(B_u) = f(E_{I_u}) = f(E_{2g}) \dots \dots \dots = f(E_{(2n-2)g})$$

Symmetry Condition

Combinations of any two (w.r.t. orientation) must appear

Inequalities



ATOM AND BOND REPRESENTATIONS FOR $C_{(4n-2)h}$ MOLECULES

Atom Site Symmetry	Atom Representation	Number of Equivalent Sets of Atoms	Symmetry of Point Complex	Bond Site Symmetry	
				Chemical Bonds	Non-Chemical Bonds
$C_{(2n+1)h}$	A'	m_o	K_h		
C_{2n+1}	$A' + A''$	m_{2n+1}	$D_{\infty h}$	$C_{(2n+1)h}$	
C_{Ih}	$A' + \sum_n E'_r$	m_h	$D_{(2n+1)h}$	C_{Ih}	$(n-1)C_{Ih}$
C_I	$A' + A'' + \sum_n E'_r + E''_r$	m	$D_{(2n+1)h}$	$C_{Ih} \cdot nC_I$	nC_I

Atom Representations

$$N = m_o + 2m_{2n+1} + (2n+1)m_h + (n+2)m$$

Chemical Condition

$$|f(A') - f(A'') - f(E'_r) + f(E''_r)| \neq 0$$

Equality

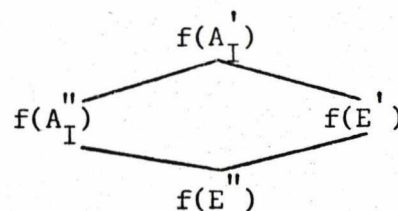
$$f(E'_1) = f(E'_2) \dots = f(E'_n)$$

$$f(E''_1) = f(E''_2) \dots = f(E''_n)$$

Symmetry Condition

Combinations of any two (w.r.t. orientation) must appear

Inequalities



ATOM AND BOND REPRESENTATIONS FOR $C_{(2n+1)h}$ MOLECULES

Atom Site Symmetry	Atom Representations	Number of Equivalent Sets of Atoms	Symmetry of Point Complex	Bond Site Symmetry	
				Chemical Bonds	Non-Chemical Bonds
C_{4nh}	A_g	m_o	K_h		
C_{4n}	$A_g + A_u$	m_{4n}	$D_{\infty h}$	C_{4nh}	
C_{Ih}	$A_g + B_g + \sum_{n-1} E_{2rg} + \sum_n E_{(2n-1)u}$	m_h	D_{4nh}	C_{Ih}	$C_{2h}, (2n-2)C_{Ih}$
C_I	$A_g + A_u + B_g + B_u + \sum_{2n-1} E_{rg} + E_{ru}$	m	D_{4nh}	C_{Ih}, C_I	$C_2, S_2, (4n-3)C_I$

Atom Representations

$$N = m_o + 2m_{4n} + (4n)m_h + (8n)m$$

Chemical Condition

$$I \gg f(A_g) - f(A_u) - f(B_g) + f(B_u) \gg 0$$

Equality

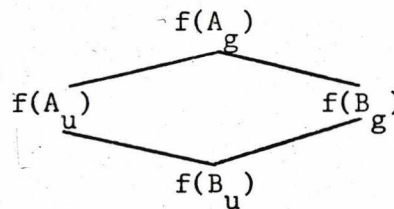
$$f(B_g) = f(E_{Iu}) = f(E_{2g}) \dots = f(E_{(2n-1)u})$$

$$f(B_u) = f(E_{Ig}) = f(E_{2u}) \dots = f(E_{(2n-1)g})$$

Symmetry Condition

Combinations of any two (w.r.t. orientation) must appear

Inequalities



ATOM AND BOND REPRESENTATIONS FOR C_{4nh} MOLECULES

Atom Site Symmetry	Atom Representation	Number of Equivalent Sets of Atoms	Symmetry of Point Complex	Bond Site Symmetry	
				Chemical Bonds	Non-Chemical Bonds
$C_{(4n-2)v}$	A_I	m_o	K_h		
C_{Iv}	$A_I + B_I + \sum_{2n-2} E_r$	m_v	$D_{\infty h} (n=I)$ $D_{(4n-2)h} (n \neq I)$	$C_{2v} (n=I)$ $C_{Id} (n \neq I)$	$(n-I)C_{Iv}, (n-2)C_{Id}$ $C_{2v} (n \neq I)$
C_{Id}	$A_I + B_2 + \sum_{2n-2} E_r$	m_d	$D_{\infty h} (n=I)$ $D_{(4n-2)h} (n \neq I)$	$C_{2v} (n=I)$ $C_{Iv} (n \neq I)$	$(n-I)C_{Id}, (n-2)C_{Iv}$ $C_{2v} (n \neq I)$
C_I	$A_I + A_2 + B_I + B_2 + 2\sum_{2n-2} E_r$	m	$D_{(4n-2)h}$	C_{Id}, C_{Iv}	$(2n-2)C_{Iv}, (2n-2)C_{Id}$ $(2n-2)C_I, C_2$

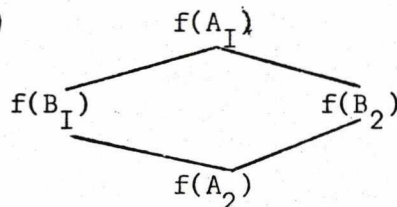
Atom Representations

$$N = m_o + (4n-2)m_v + (4n-2)m_d + (8n-4)m$$

Equality

$$f(B_I) + f(B_2) = f(E_I) = f(E_2) \dots \dots \dots = f(E_{2n-2})$$

Inequalities



Chemical Condition

$$I \gg f(A_I) + f(A_2) - f(B_I) - f(B_2) \gg 0$$

Symmetry Condition

Combinations of any two (w.r.t. orientation) must appear

ATOM AND BOND REPRESENTATIONS FOR $C_{(4n-2)v}$ MOLECULES

Atom Site Symmetry	Atom Representation	Number of Equivalent Sets of Atoms	Symmetry of Point Complex	Bond Site Symmetry	
				Chemical Bonds	Non-Chemical Bonds
$C_{(2n+1)v}$	A_I	m_o	K_h		
C_{Ih}	$A_I + \sum_n E_r$	m_h	$D_{(2n+1)h}$	C_{Ih}	$(n-1)C_{Ih}$
C_I	$A_I + A_2 + 2 \sum_n E_r$	m	$D_{(2n+1)h}$	$2C_{Ih}$	$(2n-1)C_I, C_{Ih}$

Atom Representations

$$N = m_o + 2n + 1m_h + 4n + 2m$$

Chemical Condition

$$I \gg f(A_I) + f(A_2) - f(E) \gg 0$$

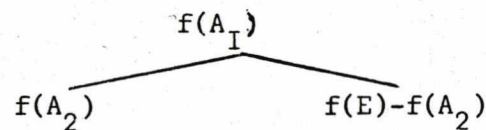
Equality

$$f(E_I) = f(E_2) = \dots \dots \dots f(E_n)$$

Symmetry Condition

Combinations of any two (w.r.t. orientation) must appear

Inequalities



ATOM AND BOND REPRESENTATIONS FOR $C_{(2n+1)v}$ MOLECULES

Atom Site Symmetry	Atom Representations	Number of Equivalent Sets of Atoms	Symmetry of Point Complex	Bond Site Symmetry	
				Chemical Bonds	Non-Chemical Bonds
C_{4nv}	A_1	m_o	K_h		
C_{Iv}	$A_1 + B_1 + \sum_{2n-1} E_r$	m_v	D_{4nh}	C_{Id}	$C_{2v}, (n-1)C_{Iv}, (n-1)C_{Id}$
C_{Id}	$A_1 + B_2 + \sum_{2n-1} E_r$	m_d	D_{4nh}	C_{Iv}	$C_{2d}, (n-1)C_{Iv}, (n-1)C_{Id}$
C_I	$A_1 + A_2 + B_1 + B_2 + 2 \sum_{2n-1} E_r$	m	D_{4nh}	C_{Id}, C_{Iv}	$C_2, nC_{Iv}, nC_{Id}, (3n-1)C_I$

Atom Representations

$$N = m_o + 4nm_v + 4nm_d + 8nm$$

Chemical Condition

$$I \gg f(A_1) - f(B_1) - f(B_2) + f(A_2) \gg 0$$

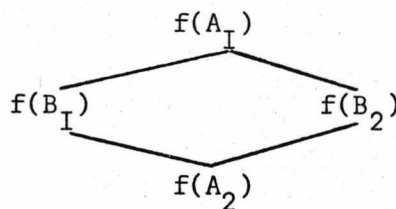
Equality

$$f(B_1) + f(B_2) = f(A_1) = f(A_2) = \dots = f(E_{2n-1})$$

Symmetry Condition

Combinations of any two (w.r.t. orientation) must appear

Inequality



ATOM AND BOND REPRESENTATIONS FOR C_{4nv} MOLECULES

Atom Site Symmetry	Atom Representations	Number of Equivalent Sets of Atoms	Symmetry of Point Complex	Bond Site Symmetry	
				Chemical Bonds	Non-Chemical Bonds
D_2	A	m_o	K_h		
C_2^z	$A+B_I$	m_z	$D_{\infty h}$	D_2	
C_2^x	$A+B_2$	m_x	$D_{\infty h}$	D_2	
C_2^y	$A+B_3$	m_y	$D_{\infty h}$	D_2	
C_I	$A+B_I+B_2+B_3$	m	D_2	C_2^x, C_2^y	C_2^z

Atom Representations

$$N = m_o + 2m_z + 2m_x + 2m_y + 4m$$

Chemical Condition

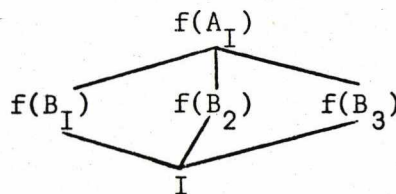
$$I \nmid 2 |f(A) - f(B_I) - f(B_2) - f(B_3)| \pmod{2} \gg 0$$

Symmetry Condition

$$m \nmid I$$

$$f(A) - f(B_I) - f(B_2) - f(B_3) + 2 |f(A) - f(B_I) - f(B_2) - f(B_3)| \pmod{2} \gg I$$

Inequalities



ATOM AND BOND REPRESENTATIONS FOR D_2 MOLECULES

Atom Site Symmetry	Atom Representation	Number of Equivalent Sets of Atoms	Symmetry of Point Complex	Bond Site Symmetry	
				Chemical Bonds	Non-Chemical Bonds
D_{2n+I}	A_I	m_o	K_h		
C_{2n+I}	$A_I + A_2$	m_{2n+I}	$D_{\infty h}$	D_{2n+I}	
C_2	$A_I + \sum_n E_r$	m_2	$D_{(2n+I)h}$	C_2	$(n-I)C_2$
C_I	$A_I + A_2 + 2 \sum_n E_r$	m	D_{2n+I}	$2C_2$	$(2n-I)C_I, C_2$

Atom Representations

$$N = m_o + 2m_{2n+I} + (2n+I)m_2 + (4n+2)m$$

Chemical Condition

$$I \geq |f(A_I) + f(A_2) - f(E)| \pmod{2} \gg 0$$

Equality

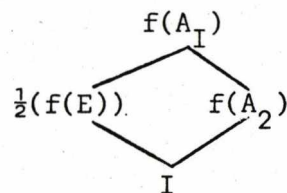
$$f(E_I) = f(E_2) = \dots \dots \dots f(E_n)$$

Symmetry Condition

$$m \gg I$$

$$\frac{1}{2}(f(E) - f(A_I) + f(A_2)) + |f(A_I) + f(A_2) - f(E)| \pmod{2} \gg I$$

Inequalities



ATOM AND BOND REPRESENTATIONS FOR D_{2n+I} MOLECULES

Atom Site Symmetry	Atom Representation	Number of Equivalent Sets of Atoms	Symmetry of Point Complex	Bond Site Symmetry	
				Chemical Bonds	Non-Chemical Bonds
D_{2n} C_{2n}	A_I $A_I + A_2$	m_0 m_{2n}	K_n $D_{\infty h}$	D_{2n}	
C_2'	$A_I + B_I + \sum_{r=1}^{n-1} E_r$	m_2'	D_{2nh}	C_2''	$D_2(C_2')$, $\frac{1}{2}(n-2)C_2''$, $\frac{1}{2}(n-1)C_2'$
C_2''	$A_I + B_2 + \sum_{r=1}^{n-1} E_r$	m_2''	D_{2nh}	C_2'	$D_2(C_2'')$, $\frac{1}{2}(n-2)C_2'$, $\frac{1}{2}(n-1)C_2''$
C_I	$A_I + A_2 + B_I + B_2 + 2\sum_{r=1}^{n-1} E_r$	m	D_{2n}	C_2', C_2''	C_2 , $(n-1)C_2'$, $(n-1)C_2''$, $(n-1)C_I$

Atom Representations

$$N = m_0 + 2m_{2n} + (2n)m_2' + (2n)m_2'' + (4n)m$$

Chemical Condition

$$I \gg |f(A_I) - f(A_2) - f(E)| \text{ mod } 2 \gg 0$$

Symmetry Condition

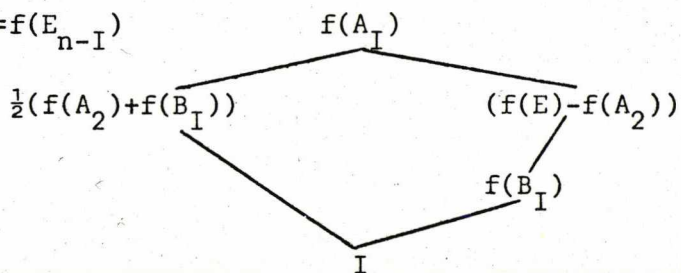
$$m \gg I$$

$$\frac{1}{2}(f(E) - f(A_I) - f(A_2)) + |f(A_I) - f(A_2) - f(E)| \text{ mod } 2 \gg I$$

Equality

$$f(B_I) + f(B_2) = f(E_I) = f(E_2) \dots \dots = f(E_{n-I})$$

Inequalities



Atom Site Symmetry	Atom Representation	Number of Equivalent Sets of Atoms	Symmetry of Point Complex	Bond Site Symmetry	
				Chemical Bonds	Non-Chemical Bonds
D_{2nd}	A_I	m_o	K_h		
C_{2nv}	A_I+B_2	m_{2nv}	$D_{\infty h}$	D_{2nd}	
C_2'	$A_I+B_I+\sum_{2n-1} E_r$	m_2	D_{4nh}	nC_{Iv}	$D_2, (n-I)C_2'$
C_{Iv}	$A_I+B_2+\sum_{2n-1} E_r$	m_v	D_{2nd}	nC_2'	$C_{2v}, (n-I)C_{Iv}$
C_I	$A_I+A_2+B_I+B_2+\sum_{2n-1} E_r$	m	D_{2nd}	nC_{Iv}, nC_2'	$C_2, nC_{Iv}, nC_2', (2n-I)C_I$

Atom Representations

$$N = m_o + 2m_{2nv} + (4n)m_2 + (4n)m_v + (8n)m$$

Chemical Condition

$$I \gg f(A_I) + f(A_2) - f(B_I) - f(B_2) \gg 0$$

Equality

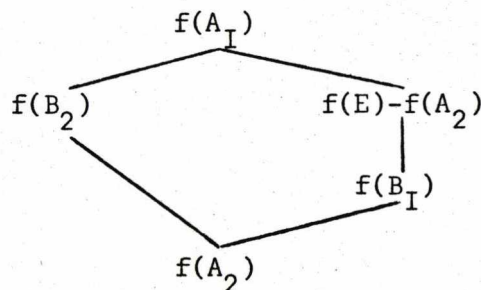
$$f(E_I) = f(E_2) \dots \dots \dots = f(E_{2n-I})$$

Symmetry Condition

$$m_v + m \gg I$$

$$f(E) - f(B_I) \gg 0$$

Inequalities



Atom Site Symmetry	Atom Representations	Number of Equivalent Sets of Atoms	Symmetry of Point Complex	Bond Site Symmetry	
				Chemical Bonds	Non-Chemical Bonds
$D_{(2n+1)d}$	A_{I_g}	m_o	K_h		
$C_{(2n+1)v}$	$A_{I_g} + A_{2u}$	$m_{(2n+1)v}$	$D_{\infty h}$	$D_{(2n+1)d}$	
C_2	$A_{I_g} + A_{2u} + \sum_n (E_{rg} + E_{ru})$	m_2	$D_{(4n+2)h}$	C_2, C_{Ih}	$C_{2h}, (n-1)C_2, (n-1)C_{Ih}$
C_{Ih}	$A_{I_g} + A_{I_u} + \sum_n (E_{rg} + E_{ru})$	m_h	$D_{(2n+1)d}$	C_2, C_{Ih}	$C_{2h}, (n-1)C_2, (n-1)C_{Ih}$
C_I	$A_{I_g} + A_{2g} + A_{I_u} + A_{2u} + 2 \sum_n (E_{rg} + E_{ru})$	m	$D_{(2n+1)d}$	$2C_2, 2C_{Ih}$	$S_2, 2nC_I, (2n-1)C_2, (2n-1)C_{Ih}$

Atom Representations

$$N = m_o + 2m_{(2n+1)v} + (4n+2)m_2 + (4n+2)m_h + (8n+4)m$$

Chemical Condition

$$I \gg (A_{I_g}) + f(A_{2g}) - f(A_{I_u}) - f(A_{2u}) \gg 0$$

Equality

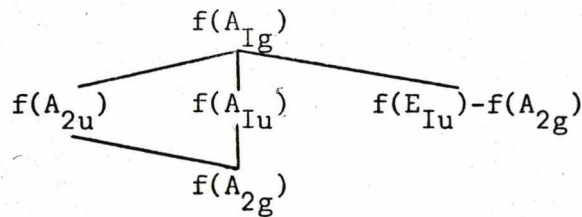
$$f(E_{I_u}) = f(E_{I_g}) = \dots = f(E_{ng}) = f(E_{nu})$$

Symmetry Condition

$$m_h + m \gg I$$

$$f(A_{I_u}) \gg I$$

Inequalities



ATOM AND BOND REPRESENTATIONS FOR $D_{(2n+1)d}$ MOLECULES

Atom Site Symmetry	Atom Representations	Number of Equivalent Sets of Atoms	Symmetry of Point Complex	Bond Site Symmetry	
				Chemical Bonds	Non-Chemical Bonds
D_{2h}	A_g	m_o	K_h		
C_{2v}^z	$A_g + B_{1u}$	m_{2z}	$D_{\infty h}$	D_{2h}	
C_{2v}^y	$A_g + B_{2u}$	m_{2y}	$D_{\infty h}$	D_{2h}	
C_{2v}^x	$A_g + B_{3u}$	m_{2x}	$D_{\infty h}$	D_{2h}	
C_{Ih}^{xy}	$A_g + B_{1g} + B_{2u} + B_{3u}$	m_h^{xy}	D_{4h}	C_{2h}^z, C_{2v}^x	C_{2v}^y
C_{Ih}^{xz}	$A_g + B_{1u} + B_{2g} + B_{3u}$	m_h^{xz}	D_{4h}	C_{2h}^y, C_{2v}^z	C_{2v}^x
C_{Ih}^{yz}	$A_g + B_{1u} + B_{2u} + B_{3g}$	m_h^{yz}	D_{4h}	C_{2h}^x, C_{2v}^y	C_{2v}^z
C_I	$A_g + A_u + B_{1u} + B_{1g} + B_{2u} + B_{2g} + B_{3u} + B_{3g}$	m	D_{2h}	$C_{Ih}^{xy}, C_{Ih}^{xz}, C_{Ih}^{yz}$	S_2, C_2^x, C_2^y, C_2^z

Atom Representations

$$N = m_o + 2m_{2z} + 2m_{2y} + 2m_x + 4m_h^{xy} + 4m_h^{yz} + 4m_h^{xz} + 8m$$

Chemical Condition

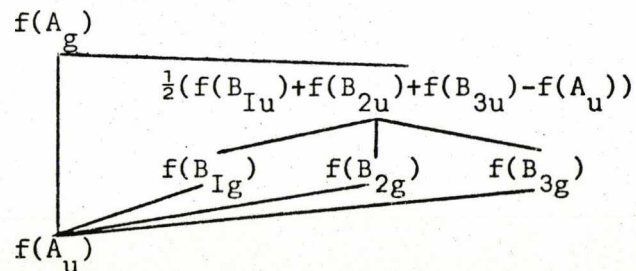
$$I \gg f(A_g) - f(A_u) + f(B_{1g}) + f(B_{2g}) + f(B_{3g}) - f(B_{1u}) - f(B_{2u}) - f(B_{3u}) \gg 0$$

Symmetry Condition

$$m \gg I$$

$$f(A_u) \gg I$$

Inequality



Atom Site Symmetry	Atom Representation	Number of Equivalent Sets of Atoms	Symmetry of Point Complex	Bond Site Symmetry	
				Chemical Bonds	Non-Chemical Bonds
$D_{(2n+1)h}$	A_I'	m_o	K_h		
$C_{(2n+1)v}$	$A_I' + A_I''$	$m_{(2n+1)v}$	$D_{\infty h}$	$D_{(2n+1)h}$	
C_{2v}	$A_I' + \sum_n E_r'$	m_{2v}	$D_{(2n+1)h}$	C_{2v}	$(n-1)C_{2v}$
C_{Iv}	$A_I' + A_2'' + \sum_n (E_r' + E_r'')$	m_v	$D_{(2n+1)h}$	C_{2v}, C_{Iv}	$nC_2, (n-1)C_{Iv}$
C_{Ih}	$A_I' + A_2' + 2\sum_n E_r'$	m_h	$D_{(2n+1)h}$	$2C_{2v}$	$nC_{Ih}, (2n-1)C_{2v}$
C_I	$A_I' + A_2' + A_I'' + A_2'' + 2\sum_n E_r' + 2\sum_n E_r''$	m	$D_{(2n+1)h}$	$C_{Ih}, 2C_{Iv}$	$(2n+1)C_2, (2n-1)C_{Iv}, 2nC_I$

Atom Representations

$$N = m_o + 2m_{(2n+1)v} + (2n+1)m_{2v} + (4n+2)m_h + (4n+2)m_v + (8n+4)m$$

Chemical Condition

$$I \gg f(A_I') + f(A_2') - f(A_I'') - f(A_2'') + f(E'') - f(E') \gg 0$$

Equality

$$f(E_1') = f(E_2') \dots \dots \dots = f(E_n')$$

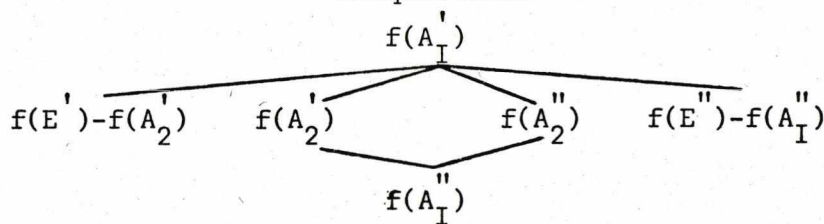
$$f(E_1'') = f(E_2'') \dots \dots \dots = f(E_n'')$$

Symmetry Condition

$$m_{2v}' + m_v' + m_h' + m \gg I$$

$$f(E') - f(A_2') \gg I$$

Inequalities



Atom Site Symmetry	Atom Representations	Number of Equivalent Sets of Atoms	Symmetry of Point Complex	Bond Site Symmetry Chemical Bonds	Non-Chemical Bonds
D_{4nh}	A_{I_g}	m_o	K_h		
C_{4nv}	$A_{I_g} + A_{2u}$	m_{4nv}	$D_{\infty h}$	D_{4nh}	
$C_{2v}(C'_2)$	$A_{I_g} + B_{I_g} + \sum_{n-1} E_{2rg} + \sum_n E_{(2r-1)u}$	m_{2v}	D_{4nh}	$C_{2d}(C''_2)$	$D_{2h}(C'_2), (n-1)C_{2v}(C'_2),$ $(n-1)C_{2d}(C''_2)$
$C_{2d}(C''_2)$	$A_{I_g} + B_{2g} + \sum_{n-1} E_{2rg} + \sum_n E_{(2r-1)u}$	m_{2d}	D_{4nh}	$C_{2v}(C'_2)$	$D_{2h}(C''_2), (n-1)C_{2v}(C'_2),$ $(n-1)C_{2d}(C''_2)$
C_{Ih}	$A_{I_g} + A_{2g} + B_{I_g} + B_{2g} +$ $2 \sum_{n-1} E_{2rg} + 2 \sum_n E_{(2r-1)u}$	m_h	D_{4nh}	$C_{2v}(C'_2),$ $C_{2d}(C''_2)$	$C_{2h}(C_2), (2n-1)C_{2v}(C_2),$ $(2n-1)C_{2d}(C''_2), (2n-1)C_{Ih}$
C_{Iv}	$A_{I_g} + A_{2u} + B_{I_g} + B_{2u} +$ $\sum_{2n-1} E_{rg} + E_{ru}$	m_v	D_{4nh}	$C_{2v}(C'_2),$ C_{Id}	$C_{2h}(C'_2), (2n-1)C_{2v}(C'_2),$ $(2n-2)C_{2v}(C'_2), (n-1)C_{Id}, nC''_2$
C_{Id}	$A_{I_g} + A_{2u} + B_{Iu} + B_{2g} +$ $\sum_{2n-1} E_{rg} + E_{ru}$	m_d	D_{4nh}	$C_{2d}(C''_2),$ C_{Iv}	$C_{2h}(C''_2), (2n-1)C_{2d}(C_2),$ $(2n-2)C_{2d}(C''_2), (n-1)C_{Iv}, nC'_2$
C_I	$A_{I_g} + A_{2g} + A_{Iu} + A_{2u} + B_{I_g} + B_{2g} +$ $B_{Iu} + B_{2u} + 2 \sum_{2n-1} E_{rg} + E_{ru}$	m	D_{4nh}	$C_{Iv}, C_{Id},$ C_{Ih}	$S_2, C_2, 2nC'_2, 2nC''_2, (2n-1)C_{Iv},$ $(2n-1)C_{Id}, (4n-2)C_I$

Atom Representations

$$N = m_o + 2m_{4v} + (4n)m_{2v} + (4n)m_{2d} + (8n)m_h + (8n)m_v + (8n)m_d + (16n)m$$

Chemical Condition

$$I \gg f(A_{I_g}) + f(A_{2g}) - f(A_{Iu}) - f(A_{2u}) + f(B_{Iu}) +$$

$$f(B_{2u}) - f(B_{I_g}) - f(B_{2g}) \gg 0$$

Equality

$$f(B_{I_g}) + f(B_{2g}) = f(E_{Iu}) = f(E_{2g}) \dots = f(E_{(2n-1)g})$$

$$f(B_{Iu}) + f(B_{2u}) = f(E_{I_g}) = f(E_{2u}) \dots = f(E_{(2n-1)u})$$

Symmetry Condition

$$m_{2v} + m_{2d} + m_h + m_v + m_d + m \gg I$$

$$f(B_{I_g}) + f(B_{2g}) - f(A_{2g}) \gg I$$

Inequalities

$$f(A_{I_g})$$

$$\frac{1}{2}(f(A_{2u}) + f(B_{I_g}) + f(B_{2g}) - f(A_{Iu}))$$

$$f(B_{Iu}) \quad f(A_{2g}) \quad f(B_{2u})$$

$$f(A_{Iu})$$

Atom Site Symmetry	Atom Representations	Number of Equivalent Sets of Atoms	Symmetry of Point Complex	Bond Site Symmetry	
				Chemical Bonds	Non-Chemical Bonds
$D_{(4n+2)h}$	A_{I_g}	m_o	K_h		
$C_{(4n+2)v}$	$A_{I_g} + A_{2u}$	$m_{(4n+2)v}$	$D_{\infty h}$	$D_{(4n+2)h}$	
$C_{2v}(C'_2)$	$A_{I_g} + B_{I_u} + \sum_n E_{2rg} + E_{(2r-1)u}$	m_{2v}	$D_{(4n+2)h}$	$C_{2d}(C''_2)$	$D_{2h}, nC_{2v}(C'_2), (n-1)C_{2d}(C''_2)$
$C_{2d}(C''_2)$	$A_{I_g} + B_{2u} + \sum_n E_{2rg} + E_{(2r-1)u}$	m_{2d}	$D_{(4n+2)h}$	$C_{2v}(C'_2)$	$D_{2h}, nC_{2d}(C''_2), (n-1)C_{2v}(C'_2)$
C_{Ih}	$A_{I_g} + A_{2g} + B_{I_u} + B_{2u} + 2 \sum_n E_{2rg} + E_{(2r-1)u}$	m_h	$D_{(4n+2)h}$	$C_{2v}(C'_2), C_{2d}(C''_2)$	$C_{2h}(C_2), 2nC_{2v}(C'_2), 2nC_{2d}(C''_2), 2nC_{Ih}$
C_{Iv}	$A_{I_g} + A_{2u} + B_{I_u} + B_{2g} + \sum_n E_{rg} + E_{ru}$	m_v	$D_{(4n+2)h}$	$C_{2v}(C'_2), C_{Id}$	$C_{2h}(C'_2), C_{2v}(C_2), nC_{Iv}, (n-1)C_{Id}, nC_2, nC_2$
C_{Id}	$A_{I_g} + A_{2u} + B_{I_g} + B_{2u} + \sum_n E_{rg} + E_{ru}$	m_d	$D_{(4n+2)h}$	$C_{2d}(C''_2), C_{Iv}$	$C_{2h}(C''_2), C_{2v}(C_2), nC_{Id}, (n-1)C_{Iv}, nC_2, nC_2$
C_I	$A_{I_g} + A_{2g} + A_{I_u} + A_{2u} + B_{I_g} + B_{2g} + B_{I_u} + B_{2u} + 2 \sum_n E_{rg} + E_{ru}$	m	$D_{(4n+2)h}$	C_{Ih}, C_{Iv}, C_{Id}	$S_2, C_2, (6n-4)C_{Iv}, (6n-4)C_{Id}, (5n-1)C_I$

Atom Representations

$$N = m_o + 2m_{(4n+2)v} + (4n+2)m_{2v} + (4n+2)m_{2d} + (8n+4)m_h + (8n+4)m_v + (8n+4)m_d + (16n+8)m$$

Chemical Condition

$$I \gg f(A_{I_g}) + f(A_{2g}) + f(B_{I_g}) + f(B_{2g}) - f(A_{I_u}) - f(A_{2u}) - f(B_{I_u}) - f(B_{2u}) \gg 0$$

Equality

$$f(E_{I_u}) = f(E_{2g}) \dots = f(E_{2nu})$$

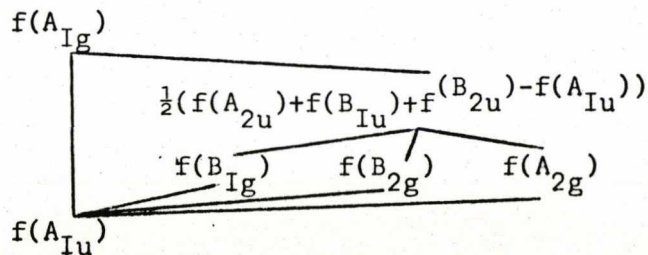
$$f(E_{I_g}) = f(E_{2u}) \dots = f(E_{2ng})$$

Symmetry Condition

$$m_{2v} + m_{2d} + m_h + m_d + m_v + m \gg I$$

$$f(B_{I_u}) + f(B_{2u}) - f(A_{2g}) \gg I$$

Inequalities



Atom Site Symmetry	Atom Representations	Number of Equivalent Sets of Atoms	Symmetry of Point Complex	Bond Site Symmetry	
				Chemical Bonds	Non-Chemical Bonds
S_{4n-2}	A_g	m_o	K_h		
C_{2n-1}	$A_g + A_u$	m_{2n-1}	$D_{\infty h}$	S_{4n-2}	
C_I	$A_g + A_u + \sum_{n-1} (E_{rg} + E_{ru})$	m	$D_{(2n-1)d}$	$S_2(n=I)$ $2C_I(n \neq I)$	$S_2(n \neq I)$ $(2n-4)C_I$

Atom Representations

$$N = m_o + 2m_{2n-1} + (4n-2)m$$

Chemical Condition

$$I \gg f(A_g) - f(A_u) \gg 0$$

Equality

$$f(E_{1g}) = f(E_{2g}) \dots = f(E_{(n-1)g}) =$$

$$f(E_{1u}) = f(E_{2u}) \dots = f(E_{(n-1)u})$$

Symmetry Condition

Combinations of any two (w.r.t. orientation) must appear

Inequalities

$$\begin{array}{c} f(A_g) \\ | \\ f(A_u) \\ | \\ f(E_g) \end{array}$$

ATOM AND BOND REPRESENTATIONS FOR S_{4n-2} MOLECULES

Atom Site Symmetry	Atom Representations	Number of Equivalent Sets of Atoms	Symmetry of Point Complex	Bond Site Symmetry	
				Chemical Bonds	Non-Chemical Bonds
S_{4n}	A	m_o	K_h		
C_{2n}	A+B	m_{2n}	$D_{\infty h}$	S_{4n}	
C_I	$A+B+\sum_{2n-1} E_r$	m	D_{2nd}	nC_I	$C_2, (n-1)C_I$

Atom Representations
 $N = m_o + 2m_{2n} + (4n)m$

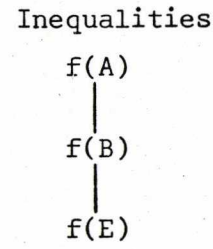
Chemical Condition
 $I \gg f(A) - f(B) \gg 0$

Symmetry Condition
 Combinations of any two (w.r.t. orientation) must appear

Equality

$$f(B) = f(E_2) = f(E_4) \dots = f(E_{2n-2})$$

$$f(E_1) = f(E_3) \dots = f(E_{2n-1})$$



ATOM AND BOND REPRESENTATIONS FOR S_{4n} MOLECULES

Atom Site Symmetry	Atom Representations	Number of Equivalent Sets of Atoms	Symmetry of Point Complex	Bond Site Symmetry	
				Chemical Bonds	Non-Chemical Bonds
T	A	m_0	K_h		
C_3	A+T	m_3	T_d	C_2	
C_2	A+E+T	m_2	O_h	C_I	D_2
C_I	A+E+3T	m	T	$2C_2, C_I$	$C_2, 3C_I$

Atom Representations

$$N = m_0 + 4m_3 + 6m_2 + 12m$$

Chemical Condition

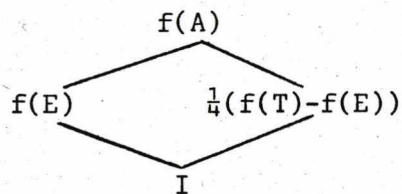
$$I \geq |f(A) + 2f(E) - f(T)| \pmod{2} \gg 0$$

Symmetry Condition

$$m \geq I$$

$$\frac{1}{2} f(T) - f(A) + |f(A) + 2f(E) - f(T)| \pmod{2} \gg I$$

Inequalities



ATOM AND BOND REPRESENTATIONS FOR TETRAHEDRAL, T, MOLECULES

Atom Site Symmetry	Atom Representation	Number of Equivalent Sets of Atoms	Symmetry of Point Complex	Bond Site Symmetry	
				Chemical Bonds	Non-Chemical Bonds
T_d	A_I	m_o	K_h		
C_{3v}	A_I+T_2	m_{3v}	T_d	C_{2v}	
C_{2v}	A_I+E+T_2	m_{2v}	O_h	C_{Ih}	D_{2d}
C_{Ih}	$A_I+E+T_I+2T_2$	m_d	T_d	$C_{2v}, 2C_{Ih}$	C_2, C_I
C_I	$A_I+A_2+2E+3T_I+3T_2$	m	T_d	$5C_{Ih}, 2C_I$	$3C_2, C_{Ih}, 5C_I$

Atom Representations
 $N = m_o + 4m_{3v} + 6m_{2v} + 12m_d + 24m$

Chemical Condition

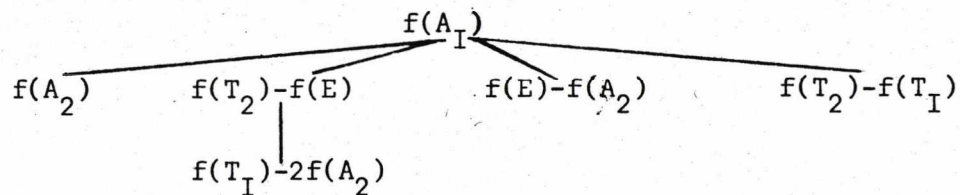
$$I \gg f(A_I) - f(A_2) + f(T_I) - f(T_2) \gg 0$$

Symmetry Condition

$$m_{3v} + m_d + m \gg I$$

$$f(T_2) - f(E) \gg I$$

Inequalities



ATOM AND BOND REPRESENTATIONS FOR TETRAHEDRAL, T_d , MOLECULES

Atom Site Symmetry	Atom Representation	Number of Equivalent Sets of Atoms	Symmetry of Point Complex	Bond Site Symmetry	
				Chemical Bonds	Non-Chemical Bonds
T_h	A_g	m_o	K_h		
C_{2v}	$A_g + E_g + T_u$	m_{2v}	O_h	C_{Ih}	D_{2h}
C_3	$A_g + A_u + T_g + T_u$	m_3	O_h	C_{Ih}	S_6, C_2
C_{Ih}	$A_g + E_g + 2T_u + T_g$	m_h	T_h	$2C_{Ih}$	C_{2h}, C_2, C_I
C_I	$A_g + A_u + E_g + E_u + 3T_g + 3T_u$	m	O_h	$2C_{Ih}, 2C_I$	$S_2, C_{Ih}, 3C_2, 6C_I$

Atom Representations

$$N = m_o + 6m_{2v} + 8m_3 + 12m_h + 24m$$

Chemical Condition

$$I \gg f(A_g) - f(A_u) + f(E_u) - f(E_g) \gg 0$$

Equality

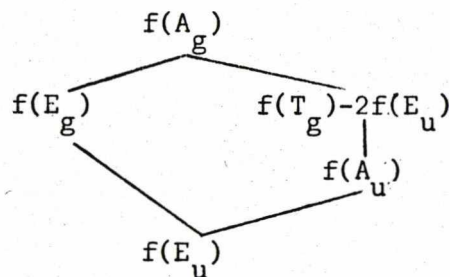
$$f(E_u) + f(T_u) = f(E_g) + f(T_g)$$

Symmetry Condition

$$m_h \gg I$$

$$f(T_g) - f(A_u) - 2f(E_u) \gg I$$

Inequalities



ATOM AND BOND REPRESENTATIONS FOR TETRAHEDRAL, T_h , MOLECULES

Atom Site Symmetry	Atom Representation	Number of Equivalent Sets of Atoms	Symmetry of Point Complex	Bond Site Symmetry	
				Chemical Bonds	Non-Chemical Bonds
O	A_I	m_O	K_h		
C_4	A_I+E+T_I	m_4	O_h	C_2'	D_4
C_3	$A_I+A_2+T_I+T_2$	m_3	O_h	C_2'	D_3, C_2
C_2'	$A_I+E+T_I+2T_2$	m_2	O_h	C_2', C_I	D_2, C_2, C_2'
C_I	$A_I+A_2+2E+3T_I+3T_2$	m	O	$5C_2', 2C_I$	$3C_2, C_2', 5C_I$

Atom Representations

$$N = m_O + 6m_4 + 8m_3 + 12m_2 + 24m$$

Chemical Condition

$$I \geq |f(A_I) - f(A_2) - f(E)| \pmod{2} \geq 0$$

Equality

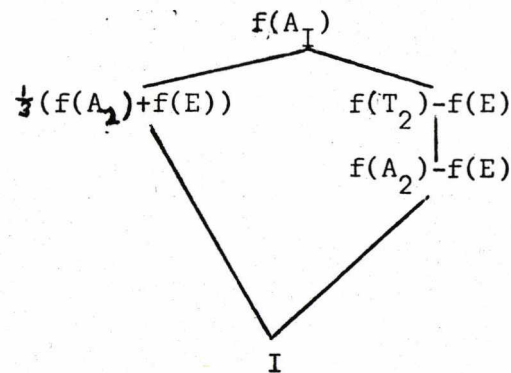
$$f(A_2) + f(E) = f(T_I)$$

Symmetry Condition

$$m \geq I$$

$$\frac{1}{2}(|f(A_I) - f(A_2) - f(E)| \pmod{2} - f(A_I) + f(A_2) + f(E)) \geq I$$

Inequalities



Atom Site Symmetry	Atom Representations	Number of Equivalent Sets of Atoms	Symmetry of Point Complex	Bond Site Symmetry	
				Chemical Bonds	Non-Chemical Bonds
O_h	A_{1g}	m_o	K_h		
C_{4v}	$A_{1g} + E_g + T_{1u}$	m_{4v}	O_h	$C_{2v}(\sigma_h \rightarrow \sigma^{xz})$	D_{4h}
C_{3v}	$A_{1g} + A_{2u} + T_{1u} + T_{2g}$	m_{3v}	O_h	$C_{2v}(\sigma_h \rightarrow \sigma^{xz})$	$D_{3d}, C_{2v}(2\sigma_d \rightarrow 2\sigma_v)$
$C_{2v}(\sigma_h \rightarrow \sigma^{xz})$	$A_{1g} + E_g + T_{1u} + T_{2g} + T_{2u}$	m_{2v}	O_h	$C_{2v}(\sigma_h \rightarrow \sigma^{xz}), C_{1d}$	$D_2(C_2 \rightarrow C_2^Z), C_{4h}, C_{2v}(2\sigma_d \rightarrow 2\sigma_v)$
C_{1h}	$A_{1g} + A_{2g} + 2E_g + T_{1g} + T_{2g} + 2T_{1u} + 2T_{2u}$	m_h	O_h	$2C_{2v}(\sigma_h \rightarrow \sigma^{xz}), C_{1d}$	$C_{2h}(C_2), 2C_{2v}(\sigma_h \rightarrow \sigma^{xz}), 2C_{2v}(2\sigma_d \rightarrow 2\sigma_v), C_2, 3C_I$
C_{1d}	$A_{1g} + A_{2u} + E_g + E_u + T_{1g} + T_{2u} + 2T_{1u} + 2T_{2g}$	m_d	O_h	$C_{2v}(\sigma_h \rightarrow \sigma^{xz}), C_{1h}, 2C_{1d}$	$C_{2h}(C_2), C_{2v}(2\sigma_d \rightarrow 2\sigma_v), C_2, 2C_2, 2C_I$
C_1	$A_{1g} + A_{2g} + A_{1u} + A_{2u} + 2E_g + 2E_u + 3T_{1g} + 3T_{2g} + 3T_{1u} + 3T_{2u}$	m	O_h	$5C_{1d}, C_{1h}, 4C_1$	$S_2, 3C_2, C_{1d}, 2C_{1h}, 6C_2, 10C_1$

Atom Representations

$$N = m_o + 6m_{4v} + 8m_{3v} + 12m_{2v} + 24m_h + 24m_d + 48m$$

Chemical Condition

$$I \gg f(A_{1g}) + f(A_{2g}) - f(A_{1u}) - f(E_g) + f(E_u) \gg 0$$

Equality

$$f(A_{2u}) + f(E_g) = f(T_{1u})$$

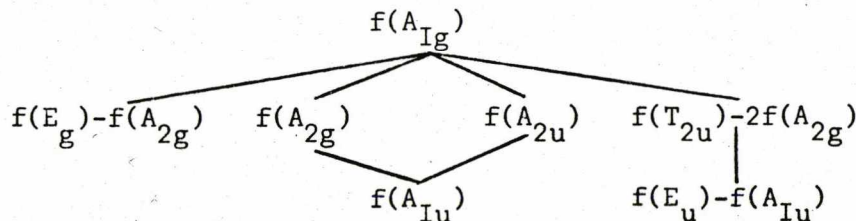
$$f(A_{2g}) + f(E_u) = f(T_{1g})$$

$$f(A_{2g}) + f(T_{2g}) = f(A_{2u}) + f(T_{2u})$$

Symmetry Condition

$$m_{4v} + m_{3v} + m_{2v} + m_h + m_d + m \gg I; f(A_{1u}) + f(A_{2u}) - f(A_{2g}) + f(E_g) - f(E_u) \gg I$$

Inequalities



Atom Site Symmetry	Atom Representation	Number of Equivalent Sets of Atoms	Symmetry of Point Complex	Bond Site Symmetry	
				Chemical Bonds	Non-Chemical Bonds
I	A	m_0	K_h		
C_5	$A+T_I+T_2+H$	m_5	I_h	C_2	D_5, C_2
C_3	$A+T_I+T_2+2G+H$	m_3	I_h	C_2, C_I	$D_3, 2D_2, C_I$
C_2	$A+T_I+T_2+2G+3H$	m_2	I_h	$2C_I$	$5D_2, 4C_I$
C_I	$A+3T_I+3T_2+4G+5H$	m	I	$3C_2, 4C_I$	$I2C_2, I8C_I$

Atom Representations

$$N = m_0 + I2m_5 + 20m_3 + 30m_2 + 60m$$

Chemical Condition

$$I \geq |f(A) - f(T_I)| \pmod{2} \geq 0$$

Equality

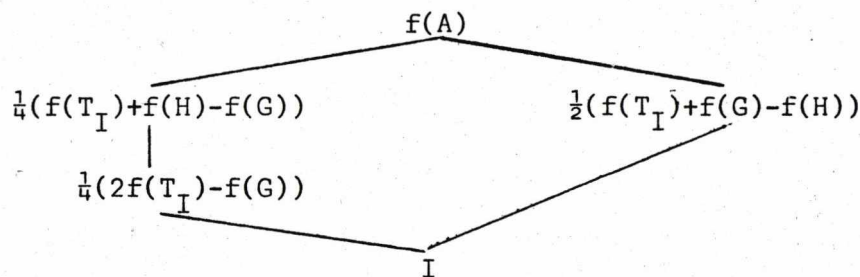
$$f(T_I) = f(T_2)$$

Symmetry Condition

$$m \geq I$$

$$\frac{1}{2} (|f(A) - f(T_I)| \pmod{2} - f(A) + f(T_I)) \geq I$$

Inequalities



ATOM AND BOND REPRESENTATIONS FOR ICOSAHEDRAL, I, MOLECULES

Atom Site Symmetry	Atom Representations	Number of Equivalent Sets of Atoms	Symmetry of Point Complex	Bond Site Symmetry	
				Chemical Bonds	Non-Chemical Bonds
I_h	A_g	m_o	K_h		
C_{5v}	$A_g + T_{Iu} + T_{2u} + H_g$	m_{5v}	I_h	C_{2v}	D_{5d}, C_{2v}
C_{3v}	$A_g + T_{Iu} + T_{2u} + G_g + G_u + H_g$	m_{3v}	I_h	C_{2v}, C_{Ih}	D_{3d}, C_{2v}, C_2
C_{2v}	$A_g + T_{Iu} + T_{2u} + G_g + G_u + 2H_g + H_u$	m_{2v}	I_h	$C_{2v}, 2C_{Ih}$	$D_{2h}, C_{2v}, 2C_2, C_I$
C_{Ih}	$A_g + T_{Ig} + T_{2g} + 2T_{Iu} + 2T_{2u} + 2G_g + 2G_u + 3H_g + 2H_u$	m_h	I_h	$C_{2v}, 2C_{Ih}, xC_I$	$2D_{2h}, 3C_{2v}, 4C_2, C_{Ih}; (10-x)C_I$
\bar{C}_I	$A_g + A_u + 3T_{Ig} + 3T_{Iu} + 3T_{2g} + 3T_{2u} + 4G_g + 4G_u + 5H_g + 5H_u$	m	I_h	yC_{2v}, zC_{Ih}, xC_I	$4D_{2h}, 9C_2, (6-y)C_{2v}, (6-z)C_{Ih}, (50-x)C_I$

Atom Representations

$$N = m_o + 12m_{5v} + 20m_{3v} + 30m_{2v} + 60m_h + 120m$$

Chemical Condition

$$I \gg f(A_g) - f(T_{Iu}) - f(A_u) + f(T_{Ig}) \gg 0$$

Equality

$$f(T_{Iu}) = f(T_{2u}); f(T_{Ig}) = f(T_{2g});$$

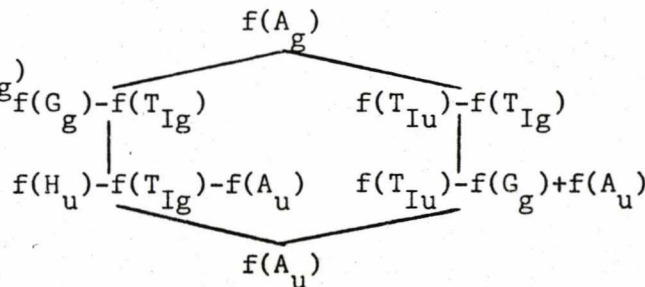
$$f(G_g) = f(G_u); f(T_{Iu}) + f(H_u) = f(T_{Ig}) + f(H_g)$$

Symmetry Condition

$$m_{5v} + m_{3v} + m_{2v} + m_h + m \gg I$$

$$f(A_u) + f(T_{Iu}) - f(T_{Ig}) \gg I$$

Inequalities



CHAPTER 3

THE REPRESENTATION GROUPS OF THE POINT GROUPS

INTRODUCTION

3.1 The purpose of this chapter is to investigate different alternative representation groups for the point groups, which lead to different equivalent sets of projective representations. The possibility of choosing a physically relevant set from these is discussed in the next two chapters.

Recently [Döring (33); Rudra (34); Hurley (35); Bradley and Cracknell (36); Janssen (37); Mozrzymas (38)], interest has been shown in the projective representations of the point groups because of their value in facilitating the determination of the representations of the non-symmorphic space groups.

There are various methods for determining these projective representations; and yet for those methods where tables have actually been published, the various results obtained were incompatible. In all of the above mentioned papers, the approach adopted has been to choose suitable factor systems rather than to calculate the representation group. It will be shown that it is both a finite and tractable problem to determine all the alternative representation groups for each point group, using an approach based on Schur's original prescription laid down in two papers in 1904 (I6), and 1907 (I7). This leads to different equivalent sets of projective representations for each point group.

All the alternative equivalent sets of projective representations can now be obtained, and it is seen that all the character systems of projective representations that have been previously published are either incomplete or erroneous or both. These sets of projective representations only differ in various phase factors for individual characters. However, these phase factors cannot be permuted between different sets, as appears

to be the case in previous papers which led to erroneous results.

3.2 THEORY OF MULTIPLICATORS AND REPRESENTATION GROUPS

Schur (17) defined a representation group, R , of a finite group, G , as an abstract group possessing an invariant subgroup, M , called the multiplier of G , which is contained in both the centre, Z , and the commutator subgroup, K , of R such that the factor group R/M is isomorphic to G . The order of M is as small as possible without being trivial, unless no non-trivial possibilities exist. The order of R is the product of the orders of G and M . The mapping of R onto R/M is a canonical epimorphism with Kernel M and image R/M , since it maps the elements of R onto the coset elements R/M . Since R/M is isomorphic to G , there is an epimorphism π from R onto G .

A representation group is therefore a central extension of G by M . In general R is not unique although M is unique for a given G . Although the elements of G can be identified with the coset representatives R/M , the construction of R is such that the multiplication rule in R for elements identified with elements of G is not the same as for those elements in the group G . G is therefore not a subgroup of R and hence R cannot have a direct or semi-direct product structure involving G and M .

One can extend the concept of a representation of a group G of elements $\{g_i\}$ to allow a multiplication law for the representative matrices, δ , of the form

$$\delta(g_i) \delta(g_j) = \omega(g_i, g_j) \delta(g_i g_j)$$

where the factor systems $\omega(g_i, g_j)$ are complex numbers of unit modules. Not every function ω can occur as a factor system because of the associative law of matrix multiplication viz:

$$[\delta(g_i) \delta(g_j)] \delta(g_k) = \delta(g_i) [\delta(g_j) \delta(g_k)]$$

$$\omega(g_i, g_j) \delta(g_i g_j) \delta(g_k) = \delta(g_i) \omega(g_j, g_k) \delta(g_j g_k)$$

$$\omega(g_i, g_j) \omega(g_i g_j, g_k) \delta(g_i g_j g_k) = \omega(g_j, g_k) \omega(g_i, g_j g_k) \delta(g_i g_j g_k)$$

Therefore the condition on ω for all $g_i, g_j, g_k \in G$ is:

$$\omega(g_i, g_j) \omega(g_i g_j, g_k) = \omega(g_j, g_k) \omega(g_i, g_j g_k)$$

These factor systems form a multiplicative Abelian group. A particular case is given by all $\omega(g_i, g_j) = 1$ when normal point group algebra is obtained.

It can be shown by the following argument that the true (or vector) representations of R correspond to either vector or generalised (or projective or ray or multiplier) representations of G . A representation matrix $\Delta(r_i)$ of R is also a representative matrix $\delta(\pi r_i)$ of G since the epimorphism π maps the element r_i of R onto the element πr_i of G . Since Δ is a true representation of R ,

$$\Delta(r_i) \Delta(r_j) = \Delta(r_i r_j)$$

but
$$\begin{aligned} \Delta(r_i) \Delta(r_j) &= \delta(\pi r_i) \delta(\pi r_j) \\ &= \delta(\pi r_i r_j) \end{aligned}$$

hence
$$\delta(\pi r_i r_j) = \Delta(r_i r_j)$$

and therefore Δ is also a representation of G .

Now let r_k be that element of R such that $\pi r_k = g_k$. Because

$$\pi(r_k r_l) = \pi r_k \cdot \pi r_l = g_k g_l = g_{kl} = \pi r_{kl}$$

$$\pi(r_{kl} r_k^{-1} r_l^{-1}) = E$$

the identity of G . This is satisfied if

$$r_k r_l = m_{kl} r_{kl}$$

where m_{kl} is an element of M which lies in the commutator subgroup K of G and which commutes with all elements of R .

Schur's lemma (I6), states that if A and B are two irreducible sets of matrices, of dimensions n and m respectively and S an $m \times n$ matrix such that $SA = BS$, then either $S = 0$ or S is non-singular and A and B are equivalent. A consequence of this is if an $n \times n$ matrix commutes with all

the elements of an irreducible set of matrices then S is a multiple of the unit matrix I . Hence $S = \omega I$ and is only valid for complex matrices.

Applying Schur's lemma to the previous calculations

$$\Delta(r_i)\Delta(r_j) = \Delta(r_i r_j) = \Delta(m_{ij} r_{ij}) = \omega(r_i, r_j)\Delta(r_{ij})$$

and since

$$\Delta(r_i) = \delta(g_i)$$

$$\delta(g_i)\delta(g_j) = \omega(g_i, g_j)\delta(g_i g_j)$$

i.e. δ is a projective representation of G .

Since $\delta(g_i g_j)$ and $\delta(g_i)\delta(g_j)$ only differ by a factor they determine the same transformation of projective space. This transformation will be unchanged if $\delta(g_i)$ is replaced by $u(g_i)\delta(g_i)$ where $u(g_i) \neq 0$ and is a complex function of the group. Two such projective representations δ and δ' are said to be associated if $\delta'(g_i) = u(g_i)\delta(g_i)$. If δ and δ' are associated the corresponding factor systems are then related by

$$\omega'(g_i, g_j) = \frac{u(g_i)u(g_j)}{u(g_i g_j)} \omega(g_i, g_j)$$

which is the condition for them to be associated.

If the δ 's are $n \times n$ matrices, $u(g_i)$ may equal any n th root of $\det \delta(g_i)$ for all $g_i \in G$, hence

$$\begin{aligned} \det [\delta'(g_i)\delta'(g_j)] &= \det [\omega'(g_i, g_j)\delta'(g_i g_j)] \\ u(g_i)^n [\det \delta(g_i)] u(g_j)^n [\det \delta(g_j)] &= \omega'(g_i, g_j)^n u(g_i g_j)^n [\det \delta'(g_i g_j)] \\ 1 &= \omega'(g_i, g_j)^n \end{aligned}$$

Therefore every factor system belonging to an n th-degree projective representation is associated to one in which all factors are the n th roots of unity.

$\omega(g_i, g_j)$ and $\omega'(g_i, g_j)$, together with all other factor systems associated to them, form a multiplicative Abelian group, $B^2(G)$ of associated

factor systems. This is an invariant subgroup of the group of all factor systems $Z^2(G)$. The factor group $Z^2(G)/B^2(G)$ is isomorphic to $H^2(G)$, the group of all classes of associated factor systems which is, in this context, the multiplier M of G .

To compare this with cohomology theory, it can be seen that the factor systems are those two-dimensional co-chains which are two-dimensional co-cycles. The sets of associated factor systems are those two-dimensional co-chains which are also co-boundaries of some one-dimensional co-chains. $H^2(G)$ is the second cohomology group of extensions of G by M .

3.3 DETERMINATION OF THE MULTIPLICATORS OF THE POINT GROUPS

In order to find the number of representation groups for the point groups G , the multiplier of G , which is unique, must be determined. The most efficient method is using an *aufbau* process, starting with the cyclic groups $C_n, S_{2n}, C_{(2n-1)h}$. The following isomorphisms exist between these groups:

$$C_{2n} \cong S_{2n}; \quad C_{4n-2} \cong S_{4n-2} \cong C_{(2n-1)h}$$

so that it is only necessary to consider the family of groups C_n . These are single-generator groups and hence Abelian. Their representation groups must therefore also be single generator Abelian groups and hence have a commutator subgroup $K = C_1$. Since the multiplier must be contained in the commutator subgroups of the representation groups, the multipliers of the cyclic groups must all be C_1 and therefore the representation group coincides with the original group and there are no projective representations.

The next family of groups to consider are the dihedral groups $D_{2n+1} \cong C_{(2n+1)v}$ of order $4n + 2$. Their multipliers may be found using the following theorem V of Schur (17).

"If p^α is the highest power of the prime number p , which divides the order g of the group G , and if the subgroups of G of order p^α are cyclic groups, the order of the multiplier of G is not divisible by p ."

Therefore the order of the groups D_{2n+1} is $2^1 \times (2n + 1)^1$. Hence the order of their multiplier is divisible by no prime number greater than 1. Their multiplier is hence C_1 .

For the groups of the family $D_{4n} \cong C_{4nv} \cong D_{2nd}$, non-trivial multipliers can be found and it will be sufficient to show that one representation group of twice their order exists to prove that the multipliers are all C_2 . The double groups D_{4n}^+ are known to have the property $D_{4n}^+/C_1^+ \cong D_{4n}$ since they are central extensions of C_1^+ by D_{4n} and since their commutator is C_n^+ , $C_1^+ (\cong C_2)$ is a possible multiplier. Since this group is of the minimal non-trivial order, the multiplier must be isomorphic to the abstract group C_2 for all possible representation groups.

The Vierergruppe, $D_2 \cong C_{2v} \cong C_{2h}$ is the first example of a direct product group as it can be factorised

$$D_2 = C_2 \times C_2$$

Before we can apply Schur's theorems we have to show that if K is the commutator subgroup of a finite group G , then the factor group G/K is always Abelian.

The commutator of an ordered pair of elements $\{g_i, g_j\}$ of a finite group G is the element $g_i^{-1} g_j^{-1} g_i g_j$. The commutator subgroup K of G is the subgroup generated by all the commutators of G . Let N be a normal subgroup of G , then the factor group G/N is Abelian if and only if N contains K ; since the elements of the cosets G/N are the cosets

$$gN = Ng \quad \forall g \in G$$

G/N is Abelian only if

$$g_i N g_i N = g_j N g_j N \quad \forall g_i, g_j \in G$$

Hence

$$Ng_i g_j = Ng_j g_i$$

$$N = g_j g_i g_j^{-1} g_i^{-1}$$

Therefore $g_j g_i g_j^{-1} g_i^{-1}$ must be an element of N and hence N must contain all commutators since g_i and g_j are any two elements of G. Thus G/K is always Abelian, and can be factorised into direct products of cyclic groups.

Theorem VI of Schur now proves that if G_1 and G_2 are two finite groups with commutator subgroups K_1 and K_2 respectively, and with quotient groups G_1/K_1 and G_2/K_2 factorised as direct products of cyclic groups of orders n_1, n_2, \dots, n_k and s_1, s_2, \dots, s_l ; then the multiplier of $G_1 \times G_2$ is the direct product of the groups M_1, M_2 and the k^2 cyclic groups of orders $\text{hcf}(n_1, s_1) \text{hcf}(n_2, s_1) \dots \text{hcf}(n_k, s_l)$ where $\text{hcf}(a, b)$ is the highest common factor of a and b.

The multiplier of D_2 is then given by

$$M(D_2) \cong M(C_2) \times M(C_2) \times C_{\text{hcf}(2,2)}$$

$$\cong C_1 \times C_1 \times C_2$$

$$\cong C_2$$

The multipliers of the tetrahedral, octahedral and icosahedral rotation groups, T, O and I respectively, may now be determined by Theorem V of Schur (17). Since apart from cyclic groups of odd order, their Sylow subgroups are respectively D_2, D_4, D_2 . These all have multipliers isomorphic to C_2 and hence if T, O and I are to have non-trivial multipliers, these must all be isomorphic to C_2 . The multiplier of the regular tetrahedral group, T_d , must also be isomorphic to C_2 since T_d is isomorphic to O.

All other remaining point groups can be regarded as direct product groups:

$$C_{2nh} \cong C_{2n} \times C_2$$

$$D_{4n+2} \cong C_{(4n+2)v} = D_{(2n+1)d} = D_{(2n+1)h} = D_{2n+1} \times C_2$$

$$D_{2nh} \cong D_{2n} \times C_2$$

$$T_h \cong T \times C_2$$

$$O_h \cong O \times C_2$$

$$I_h \cong I \times C_2$$

and hence their multipliers can be determined using Theorem VI of Schur (17).

Finally the spherical rotation group, K , is known to have a double group, K^+ , such that $K^+/C_1^+ \cong K$. This obeys the requirements for a representation group and hence the multiplier is determined to be isomorphic to C_2 . The spherical group relevant to atoms is $K_h = K \times S_2$ and contains reflection planes and the inversion. This has a direct product group structure and again using Theorem VI of Schur (17), its multiplier is also isomorphic to C_2 .

The results may be summarised as follows, where only one member of an isomorphism class is tabulated as the results for the rest of the class automatically follow.

<u>Point Group G</u>	<u>Sylow Subgroups</u>	<u>p^α</u>
D_{2n+1}	C_2, C_{2n+1}	$2^1, (2n+1)^1$
T	D_2, C_3	$2^2, 3^1$
O	D_4, C_3	$2^3, 3^1$
I	D_2, C_3, C_5	$2^2, 3^1, 5^1$

<u>Point Group $G \cong G_1 \times G_2$</u>	<u>K_1</u>	<u>G_1/K_1</u>	<u>τ_1, τ_2</u>	<u>K_2</u>	<u>G_2/K_2</u>	<u>ξ_1</u>
$D_2 \cong C_2 \times C_2$	C_1	C_2	2, -	C_1	C_2	2
$C_{2nh} \cong C_{2n} \times C_2$	C_1	C_{2n}	2n, -	C_1	C_2	2
$D_{4n+2} \cong D_{2n+1} \times C_2$	C_{2n+1}	C_2	2, -	C_1	C_2	2
$D_{2nh} \cong D_{2n} \times C_2$	C_n	$C_2 \times C_2$	2, 2	C_1	C_2	2
$T_h \cong T \times C_2$	D_2	C_3	3, -	C_1	C_2	2
$O_h \cong O \times C_2$	T	C_2	2, -	C_1	C_2	2
$I_h \cong I \times C_2$	I	C_1	1, -	C_1	C_2	2
$K_h \cong K \times C_2$	K	C_1	1, -	C_1	C_2	2

Multiplicator $\cong C_1$:

$C_n, C_{(2n-1)h}, C_{(2n-1)v}, D_{2n+1}, S_{2n}$

Multiplicator $\cong C_2$:

$C_{2nv}, C_{2nh}, D_{2n}, D_{nd}, D_{(2n+1)h}, I, I_h, K, K_h, O, T, T_h$

Multiplicator $\cong C_2 \times C_2$:

O_h

Multiplicator $\cong C_2 \times C_2 \times C_2$:

D_{2nh}

It is seen that the multiplicators for the point groups are isomorphic to C_1 or products of C_2 . However, multiplicators of other types can appear e.g. if p is a prime number, the multiplicator of the direct product groups $C_p \times C_p$ (used in describing molecules exhibiting internal rotation) are isomorphic to C_p . The simplest example of this occurrence is when considering the direct product group $C_3 \times C_3$ where the multiplicator is isomorphic to C_3 .

It should be noted that the above determination of the multiplicator as a means of finding the second cohomology group is a labour-saving method

for those problems involving the extensions of a group by its multiplier and is far simpler than direct application of cohomology theory.

3.4 DETERMINATION OF THE MAXIMUM NUMBER OF REPRESENTATION GROUPS

The determination of the number of representation groups is usefully preceded by the determination of the maximum possible number of such groups using Theorems I and II of Schur (17). To apply these theorems we need to know the multipliers, M , determined in the previous section and the commutator subgroups, K , of the point groups G . The quotient groups G/K which have been shown to be always Abelian are factorised in terms of cyclic groups $C_{\epsilon_1} \times C_{\epsilon_2} \times C_{\epsilon_3} \dots$ where the orders $\epsilon_1, \epsilon_2 \dots$ are the integers referred to by Schur as the invariants of the quotient group. The multiplier is likewise factorised and its invariants denoted by $e_1, e_2 \dots$. Schur (Theorem I) then proved that the maximum number of representation groups, n_{\max} , is given by the product of all possible highest common factors of the type $\text{hcf}(\epsilon_i, e_j)$. When G is a complete group as for example the groups T_d and O , this maximum number is the actual number of representation groups. If the orders of the factor group G/K and M have no factors in common then G has only one representation group (Schur's Theorem II). This case happens particularly when $G = K$, as in the case for the point groups I and K , when there is only one representation group irrespective of the multiplier. The results may be summarised in the following table where n is the actual number of representation groups determined in the following section.

<u>G</u>	<u>K</u>	<u>G/K</u>	<u>M</u>	<u>n^{max}</u>	<u>n</u>
C_{2n-1}	C_1	C_{2n-1}	C_1	1	1
$C_{2n}, S_{2n}, C_{nh}(\text{nodd})$	C_1	C_{2n}	C_1	1	1
C_{2nh}	C_1	$C_{2n} \times C_2$	C_2	4	2
$D_{2n-1}, C_{(2n-1)v}$	C_{2n-1}	C_2	C_1	1	1
$D_{2n}, C_{2nv}, D_{nd}, D_{nh}(\text{nodd})$	C_n	$C_2 \times C_2$	C_2	4	$\begin{cases} 2, n = 1 \\ 3, n \neq 1 \end{cases}$
D_{2nh}	C_n	$C_2 \times C_2 \times C_2$	$C_2 \times C_2 \times C_2$	512	$\begin{cases} 1, n = 1 \\ 2, n \neq 1 \end{cases}$
T	D_2	C_3	C_2	1	1
T_d, O	T	C_2	C_2	2	2
T_h	D_2	$C_2 \times C_3$	C_2	2	2
O_h	T	$C_2 \times C_2$	$C_2 \times C_2$	16	4
I	I	C_1	C_2	1	1
I_h	I	C_2	C_2	2	2
K	K	C_1	C_2	1	1
K_h	K	C_2	C_2	2	2

3.5 DETERMINATION OF THE EXACT NUMBER OF ALTERNATIVE REPRESENTATION GROUPS

The determination of the actual number, n , of non-isomorphic representation groups of a given group, G , requires an examination of the n_{max} possibilities to see if they lead to groups and then what isomorphisms exist between them. This can be done by examining the generating relations of a given group i.e. examination of the behaviour of a minimum set of elements of the group which specify the behaviour of all elements of that group. The process can be facilitated by considering first the representation groups, R , of point groups, G , which can be specified by two

generators and then using these as a basis in a composition series for considering those groups which must be specified by three generators. then stepwise to those groups which are conveniently specified by four or five generators.

Let us consider a group G specified by two generators A and B such that $A^m = B^n = E$ and $BA = A^x B^y$. A representation group R for G must be specified in terms of two generators, P and Q such that $P^\lambda = Q^\mu = E$, and $QP = P^\xi Q^\eta$. The order of G is ℓm since for all point groups in question $A^{\frac{1}{2}\ell} \neq B^{\frac{1}{2}m}$ and hence the order required for R is $2\ell m$ since the multiplier for all two-generator point groups is of order 2. Hence, if $P^{\frac{1}{2}\lambda} \neq Q^{\frac{1}{2}\mu}$, $2\ell m = \lambda\mu$ i.e. $\lambda = 2\ell, \mu = m$ or $\lambda = \ell, \mu = 2m$. If however, $P^{\frac{1}{2}\lambda} = Q^{\frac{1}{2}\mu}$ then $2\ell m = \frac{1}{2}\lambda\mu$ i.e. $\lambda = 2\ell, \mu = 2m$, [cases such as $\lambda = 4\ell, \mu = m$ are excluded since these would not correspond to a multiplier of order 2]. Considering now The relation $BA = A^x B^y$, the corresponding relation $QP = P^\xi Q^\eta$ in the representation group can permit different combinations of values of ξ and η according to the values of λ and μ . The results can be summarized as follows:

Label	Generating Relations in R	Multiplier	Commutators of R	
			$K \begin{pmatrix} x=I \\ y=I \end{pmatrix}$	$K \begin{pmatrix} x=2n-I \\ y=I \end{pmatrix}$
ρ_1	$P^{2\ell} = Q^m = E; QP = P^x Q^y$	$\{E, P^\ell\}$	E	n even: $P^{2\ell} = E$ n odd: $(P^4)^{\frac{1}{2}\ell} = E$
ρ_2	$P^{2\ell} = Q^m = E; QP = P^{x+\ell} Q^y$	$\{E, P^\ell\}$	$(P^2)^\ell = E$	$P^{2\ell} = E$
ρ_3	$P^\ell = Q^{2m} = E; QP = P^x Q^y$	$\{E, Q^m\}$	E	$P^\ell = E$
ρ_4	$P^\ell = Q^{2m} = E; QP = P^x Q^{y+m}$	$\{E, Q^m\}$	$(Q^2)^m = E$	n even: $(P^2 Q^2)^\ell = E$ n odd: $P^\ell = (Q^2)^{\frac{1}{2}\ell} = E$
ρ_5	$P^{2\ell} = Q^{2m} = E; QP = P^x Q^y$	$\{E, P^\ell = Q^m\}$	E	n even: $(P^2 Q^2)^\ell = E$ n odd: $(P^4)^{\frac{1}{2}\ell} = E$
ρ_6	$P^{2\ell} = Q^{2m} = E; QP = P^{x+\ell} Q^y$	$\{E, P^\ell = Q^m\}$	$(P^2)^\ell = E$	$P^{2\ell} = E$
ρ_7	$P^{2\ell} = Q^{2m} = E; QP = P^x Q^{y+m}$	$\{E, P^\ell = Q^m\}$	$(P^2)^\ell = E$	$P^{2\ell} = E$
ρ_8	$P^{2\ell} = Q^{2m} = E; QP = P^{x+\ell} Q^{y+m}$	$\{E, P^\ell = Q^m\}$	E	n even: $P^{2\ell} = E$ n odd: $P^{2\ell-4} = E$

Of the eight possibilities it may be noted that $\rho_5 = \rho_8$ and $\rho_6 = \rho_7$ since for these groups, the invariant element $P^\ell = Q^m$. Among the relevant point groups, we always have $y = 1$ and either $x = 1$ (for the C_{2nh} family) or $x = 2n-1$ (for the D_{2n} family). For these two cases, the generating relations of the commutator subgroups of the representation groups are listed. Comparison with the elements of the multiplier shows that for the C_{2nh} groups, ρ_2 and ρ_6 are possible representation groups when ℓ is even which is the case since $\ell = 2n$, and ρ_4 is a representation group when m is even, which is satisfied since $m = 2$ for the C_{2nh} point groups. In fact ρ_2 and ρ_6 are isomorphic since different choices of generators will lead to the two different formulations of the group. There are thus only two different representation groups for each group of the C_{2nh} family.

In the case of the D_{2n} groups, comparison of commutator subgroups and multipliers shows that when n is even, ρ_1, ρ_2, ρ_5 and ρ_6 are possible representation groups while when n is odd, ρ_2, ρ_4 and ρ_6 are the possible representation groups. Detailed examination of the structure of these groups shows that when n is even, ρ_5 is isomorphic to ρ_1 and hence there will be three representation groups, albeit of different types, for each value of $n \neq 1$. When $n = 1$, $\rho_4 = \rho_2$ and so there are only two non-isomorphic representation groups viz ρ_2 and ρ_6 .

This approach may be extended to the remaining point groups by considering the following composition series in which each group is a normal subgroup of the following group and hence by addition of one generator and a specification of its multiplicative properties with the other generators, one can arrive at the next group in the series.

$$D_2 \longrightarrow T \longrightarrow T_h$$

$$D_2 \longrightarrow T \longrightarrow O(\cong Td) \longrightarrow Oh$$

$$D_2 \longrightarrow T \longrightarrow I \longrightarrow Ih$$

Now considering the tetrahedral rotation group, T, this may be specified by three generators viz

$$D_2 : A^2=B^2=E; BA=AB$$

$$T : A^2=B^2=E; BA=AB; C^3=E; CA=BC; CB=ABC$$

Using the fact already established that there are only two possible representation groups for D_2 , the behaviour of the corresponding two generators for the representation group of T are determined. The results for the number of possibilities for the representation group of T are shown in the following table.

<u>Generators of $R_1(D_2)$</u>	<u>Remaining Generators for R(T)</u>	<u>Label</u>
$A^4=B^2=E$ $BA=A^3B$	$C^3=E; CA=BC; CB=ABC$	ρ_1
	$C^3=E; CA=BC; CB=A^3BC$	ρ_2
	$C^3=E; CA=A^2BC; CB=ABC$	ρ_3
	$C^3=E; CA=A^2BC; CB=A^3BC$	ρ_4
<u>Generators of $R_2(D_2)$</u>		
$A^4=B^4=E$ $A^2=B^2$ $BA=A^3B$	$C^3=E; CA=BC; CB=ABC$	ρ_5
	$C^3=E; CA=A^2BC; CB=ABC$	ρ_6
	$C^3=E; CA=BC; CB=A^3BC$	ρ_7
	$C^3=E; CA=A^2BC; CB=A^3BC$	ρ_8

Consideration of the doubling of the order of the three fold element in the representation group results in isomorphisms to the above table of groups.

On detailed examination of the above results it is found that ρ_1, ρ_2, ρ_3 and ρ_4 do not constitute a group. The remaining relationships are all non-isomorphic to each other, resulting in only one possible representation group for T.

We can now consider the four-generator group, T_h , which has the generating relations:

$$A^2=B^2=C^3=I^2=E; \quad BA=AB; \quad CA=BC; \quad CB=ABC$$

$$IA=AI; \quad IB=BI; \quad IC=CI$$

using the generators of $R(T)$ as a basis. The following table shows the possible relationships that the fourth generator I has with the generators of $R(T)$.

ρ_1	$I^2=E; \quad IA=AI; \quad IB=BI; \quad IC=CI$
ρ_2	$I^2=E; \quad IA=A^3I; \quad IB=BI; \quad IC=CI$
ρ_3	$I^2=E; \quad IA=AI; \quad IB=A^2BI; \quad IC=CI$
ρ_4	$I^2=E; \quad IA=A^3I; \quad IB=A^2BI; \quad IC=CI$
ρ_5	$I^4=E; \quad IA=AI; \quad IB=BI; \quad IC=CI$
ρ_6	$I^4=E; \quad IA=A^3I; \quad IB=BI; \quad IC=CI$
ρ_7	$I^4=E; \quad IA=AI; \quad IB=A^2BI; \quad IC=CI$
ρ_8	$I^4=E; \quad IA=A^3I; \quad IB=A^2BI; \quad IC=CI$

It is then found that ρ_1, ρ_2, ρ_3 and ρ_4 are all isomorphic and ρ_5, ρ_6, ρ_7 and ρ_8 are all isomorphic resulting in only two possibilities for the representation groups of T_h .

The next four generator group to be considered is the octahedral rotation group O specified by:

$$A^2=B^2=C^3=D^2=E; \quad BA=AB; \quad CA=BC; \quad CB=ABC;$$

$$DA=BD; \quad DB=AD; \quad DC=C^2D$$

using $R(T)$ as a basis. The following results are obtained:

$$\begin{aligned}
 \rho_1 & D^2=E; DA=BD; DB=AD; DC=C^2D \\
 \rho_2 & D^2=E; DA=A^2BD; DB=AD; DC=C^2D \\
 \rho_3 & D^2=E; DA=A^2BD; DB=A^3D; DC=C^2D \\
 \rho_4 & D^2=E; DA=BD; DB=A^3D; DC=C^2D \\
 \rho_5 & D^4=E; DA=BD; DB=AD; DC=C^2D \\
 \rho_6 & D^4=E; DA=A^2BD; DB=A^3D; DC=C^2D \\
 \rho_7 & D^4=E; DA=BD; DB=A^3D; DC=C^2D \\
 \rho_8 & D^4=E; DA=A^2BD; DB=AD; DC=C^2D
 \end{aligned}$$

If it is found that ρ_2, ρ_4, ρ_7 and ρ_8 do not form a group, ρ_1 is isomorphic to ρ_3 and ρ_5 is isomorphic to ρ_6 . Therefore there are only two possibilities for the representation group of the octahedral group O.

The final four-generator point group is the icosahedral rotation group I, specified by:

$$A^2=B^2=C^3=F^5=E; \quad BA=AB; CA=BC; CB=ABC; FA=AF^4; FB=BC^2F^2; FC=C^2F^4$$

and again R(T) can be used as a basis for finding the representation groups of the icosahedron. The following table shows the possibilities for the behaviour of the fourth generator in R(I).

$$\begin{aligned}
 \rho_1 & F^5=E; FA=AF^4; FB=BC^2F^2; FC=C^2F^4 \\
 \rho_2 & F^5=E; FA=A^3F^4; FB=BC^2F^2; FC=C^2F^4 \\
 \rho_3 & F^5=E; FA=AF^4; FB=A^2BC^2F^2; FC=C^2F^4 \\
 \rho_4 & F^5=E; FA=A^3F^4; FB=A^2BC^2F^2; FC=C^2F^4 \\
 \rho_5 & F^5=E; FA=AF^4; FB=BC^2F^2; FC=A^2C^2F^4 \\
 \rho_6 & F^5=E; FA=A^3F^4; FB=BC^2F^2; FC=A^2C^2F^4 \\
 \rho_7 & F^5=E; FA=AF^4; FB=BC^2F^2; FC=A^2C^2F^4 \\
 \rho_8 & F^5=E; FA=A^3F^4; FB=BC^2F^2; FC=A^2C^2F^4
 \end{aligned}$$

As with the representation group for T, doubling the order of the five-fold generator results only in isomorphisms to the above groups. It is found that the only generating relations in the previous table that constitute a group is given by ρ_8 . Hence, there is only one representation group for the icosahedral group I.

The determination of the representation groups for the five generator groups, the icosahedron, I_h , and the octahedron, O_h , proceeds in exactly the same way as for the four-generator groups. This is relatively straightforward, even for the case of O_h where the multiplier is of increased order. Therefore it does not appear to be necessary to tabulate the detailed calculations for these cases.

The groups of the family D_{2nh} , however, where the multiplier is of order eight, requires an approach similar to that for two generators. The D_{2nh} family is specified by the generating relationships:

$$A^{2n}=B^2=C^2=E; BA=A^{2n-1}B; CA=AC; CB=BC$$

Since this group is being extended by a group of order eight it would be very tedious to have to enumerate all the possible generating relationships for the representation groups, R. However, the commutator subgroup, K, of R must contain the multiplier of G. Then by investigation of the commutator elements for each generating relationship, the allowable commutator subgroups containing M, will be the sum and the products of each set of commutator elements. It was found that of the 512 possibilities found by Schur, only 64 need be considered because of the symmetrical nature of the extension i.e. the extension is by the group $\cong C_2 \times C_2 \times C_2$ not C_8 hence it follows that each generator may be doubled in order. Other possibilities of non-symmetrical change to the group structure may be ignored. Of these 64 possibilities only 14 have allowable commutator subgroups that contain the multiplier, and only two are non-isomorphic for any particular value of n; except when $n=1$ when there is only one

non-isomorphic representation group.

Finally the spherical rotation groups K and K_h need to be considered. It has already been mentioned that the double group K^+ is a possible representation group and it is the only representation group in accordance with Theorem II of Schur (17). Similarly the group K_h has a direct product group structure and it has been shown that the maximum number of representation groups is two. The double group K_h^+ is one representation group of K_h , the second being one in which a non-invariant four-fold element and its inverse map onto the inversion in K_h .

The simplest group whose multiplier is not isomorphic to C_1 or products of C_2 is the direct product group $C_3 \times C_3$ with multiplier $\cong C_3$. On application of Theorem I of Schur (17) it is found that the maximum number of representation groups is three. In fact of these only two are non-isomorphic, having the following generating relations:

$$C_3 \times C_3 : A^3 = B^3 = E; BA = AB$$

$$R_1(C_3 \times C_3) : A^9 = B^3 = E; BA = A^4 B$$

$$R_2(C_3 \times C_3) : A^9 = B^9 = E; A^3 = B^3; BA = A^4 B$$

3.6 THE CHARACTER TABLES FOR ALL REPRESENTATION GROUPS OF THE POINT GROUPS

The following character tables of the representation groups are listed here for the first time. These supersede all previous compilations of projective representations, either because they do not list more than one possible set of projective representations (Döring 1959; Hurley 1965) or additionally they contain demonstrable errors (e.g. the D_{2h} tables of Janssen (1973) and Mozyrzymas (1975)), usually in an incorrect choice of phase of the characters. The advantage of using the full representation group rather than a set of characters of the projective representations of the point group is that R is a genuine group and hence operations involving

the projective representations, such as the symmetrization of powers, can be performed without need for any additional algebraic formulations. The tables are also useful as they contain all central extensions of G by M and hence may assist in physical problems where group extensions are needed, as well as enlarging the categories of abstract groups for which character tables are available.

The tables are presented in the format customary to molecular physics in which $\{1,2,3,4,5,6,8,12\}$ -dimensional representations are denoted by the letters $\{A,E,T,G,H,I,K,O\}$ of the Mulliken-Placzek system irrespective of whether the degeneracy is separable (Frobenius, ³⁹) or not. The complex conjugate components of separably-degenerate representations have been denoted by the superscripts $+$ and $-$. The elements of the multiplier, M , have been placed at the beginning and, since they coincide with the centre of the representation group, their characters are \pm those for the identity element. The vector representations have positive characters for all elements of the multiplier, while the projective representations have half of these characters positive and half negative. The different classes of representations have been called ω -representations by Bradley and Backhouse (⁴⁰) and are denoted by subscripts $\alpha, \beta, \alpha\beta$, etc. (except for those groups with multiplier where the well-known double group is a representation group): in such cases the double-valued representations denoted by half-integral subscripts are the projective or α -representations. The elements of the representation group have been described in terms of generators $P,Q,R \dots$ and the elements of the point group (described in terms of generators $A,B,C \dots$) to which these correspond are indicated in the relevant columns below the characters. The composition of a class has been denoted by a symbol of type $X\epsilon_x$ which means that it contains X elements of order x . Inverse pairs of elements have been collected on the same horizontal line and the relationship between the generators for both R and G have been collected on the right-hand side.

The abstract generators of the point groups may be identified by means of the following table.

G	A	B	C	D	F	I
C_{2nh}	C_{2n}	σ_h				
C_{2nv}	C_2	σ_v				
D_{2n}	C_{2n}	C_2'				
D_{nd}	S_{2n}	σ_d				
$D_{(2n+1)h}$	S_{2n+1}	σ_v				
D_{2nh}	C_{2n}	σ_v				
T	C_2^z	C_2^x	σ_h			
T_h	C_2^z	C_2^x	C_3^{xyz}			S_2
T_d	C_2^z	C_2^x	C_3^{xyz}	σ_d^{zx}		
O	C_2^z	C_2^x	C_3^{xyz}	$C_2'^{zx}$		
O_h	C_2^z	C_2^x	C_3^{xyz}	$C_2'^{zx}$		
I	C_2^z	C_2^x	C_3^{xyz}		$C_5^{(\phi)\phi^{-1}}$	S_2
I_h	C_2^z	C_2^x	C_3^{xyz}		$C_5^{(\phi)\phi^{-1}}$	S_2

It may be mentioned that not only do these tables contain the first correct characters for the projective representations of D_{2h} but also they consider the icosahedral groups for the first time.

	$1 \leq p \leq n$	$1 \leq p \leq n-1$	$1 \leq p \leq 2n-1$	8n elements
$R_1(C_{2nh})$	$1 \leq p \leq n$ $2\epsilon_{2n/hcf(n, 2p-1)}^{1\epsilon_n/hcf(n, p)}$	$1 \leq p \leq n-1$ $1\epsilon_{lcm(n, 2)}$	$1 \leq p \leq 2n-1$ $2\epsilon_{4lcm(2n, p)}^{2\epsilon_{2n/hcf(2n, p)}}$	$P^{2n} = Q^4 = E$ $QP = PQ^3$
E	Q^2	P^2P	P^2PQ^2	P^3 P^3Q
A _g	1	1	1	1
B _g	1	1	1	$(-1)^{n+p}$
A _u	1	1	1	-1
B _u	1	1	1	$(-1)^{n+p+1}$
E _{lg} ⁺	1	$i\ell(2p-1)\pi/n$	$2i\ell p\pi/n$	$-e^{-i\ell p\pi/n}$
E _{lg} ⁻	1	$-i\ell(2p-1)\pi/n$	$-2i\ell p\pi/n$	$-e^{-i\ell p\pi/n}$
E _{lu} ⁺	1	$i\ell(2p-1)\pi/n$	$2i\ell p\pi/n$	$e^{i\ell p\pi/n}$
E _{lu} ⁻	1	$-i\ell(2p-1)\pi/n$	$-2i\ell p\pi/n$	$e^{-i\ell p\pi/n}$
n even;	2	-2	2	0
E _{1/2n}	2	2	-2	0
E _n	2	2	-2	0
G _l ⁺	2	$2e^{2\pi\ell i/n}$	$-2e^{2\pi\ell i/n}$	0
G _l ⁻	2	$2e^{-2\pi\ell i/n}$	$-2e^{-2\pi\ell i/n}$	0
C _{2nh}	E	A ^{2p-1}	A ^{2p}	B
				A ²ⁿ = B ² = E
				BA = AB

$\mathcal{R}_2(C_{2nh})$	$1 \leq p \leq n$		$\left\{ \begin{matrix} 1 \leq p \leq n-1 \\ n+1 \leq p \leq 2n-1 \end{matrix} \right\}$		$1 \leq p \leq 2n-1$		8n elements		
	$1\epsilon_1$	$1\epsilon_2$	$2\epsilon_{4n/\text{hcf}(n, 2p-1)}$	$2\epsilon_{2n/\text{hcf}(2n, p)}$	$2\epsilon_4$	$2\epsilon_{\text{lcm}(\frac{4n}{\text{hcf}(4n, p)}, 4)}$			
	E	P^{2n}	$P^{2n+2p-1}$ P^{2p-1}	P^{2p}	$P^{2n}Q$ Q	$P^{2n+p}Q$ P^pQ	$P^{4n}=Q^4=E$ $P^{2n}=Q^2$ $QP=P^{2n+1}Q$		
A_g	1	1	1	1	1	1	} $\alpha=+1$		
B_g	1	1	-1	1	$(-1)^n$	$(-1)^{n+p}$			
A_u	1	1	1	1	-1	-1			
B_u	1	1	-1	1	$(-1)^{n+1}$	$(-1)^{n+p+1}$			
$1 \leq \ell \leq n-1; E_{\ell g}$	$\left\{ \begin{matrix} E_{\ell g}^+ \\ E_{\ell g}^- \end{matrix} \right.$	1	1	$e^{i\ell(2p-1)\pi/n}$	$e^{2i\ell p\pi/n}$	$(-1)^\ell$		$-e^{i\ell p\pi/n}$	
		1	1	$e^{-i\ell(2p-1)\pi/n}$	$e^{-2i\ell p\pi/n}$	$(-1)^\ell$		$-e^{-i\ell p\pi/n}$	
$1 \leq \ell \leq n-1; E_{\ell u}$	$\left\{ \begin{matrix} E_{\ell u}^+ \\ E_{\ell u}^- \end{matrix} \right.$	1	1	$e^{i\ell(2p-1)\pi/n}$	$e^{2i\ell p\pi/n}$	$(-1)^{\ell+1}$		$e^{i\ell p\pi/n}$	
		1	1	$e^{-i\ell(2p-1)\pi/n}$	$e^{-2i\ell p\pi/n}$	$(-1)^{\ell+1}$		$e^{-i\ell p\pi/n}$	
n odd;	E	2	-2	0	$2(-1)^p$	0		0	} $\alpha=-1$
$1 \leq \ell \leq \frac{1}{2}n; G_\ell$	$\left\{ \begin{matrix} G_\ell^+ \\ G_\ell^- \end{matrix} \right.$	2	-2	0	$2e^{ip(2\ell-1)\pi/n}$	0		0	
		2	-2	0	$2e^{-ip(2\ell-1)\pi/n}$	0	0		
C_{2nh}	E		A^{2p-1}	A^{2p}	B	A^pB	$A^{2n}=B^2=E$ $BA=AB$		

	$1 \leq p \leq 2n-1$					
	$1\epsilon_1$	$1\epsilon_2$	$2\epsilon_{4n/\text{hcf}(4n,p)}$	$2n\epsilon_4$ $0 \leq q \leq 2n-1$	$2n\epsilon_4$ $0 \leq q \leq 2n-1$	8n elements
$\mathcal{R}_{1(D_{2n})}$	E	P^{2n}	P^{4n-p} P^p	$P^{2q}Q$	$P^{2q+1}Q$	$P^{4n}=Q^4=E; P^{2n}=Q^2$ $QP=P^{4n-1}Q$
A_1	1	1	1	1	1	} $\alpha=+1$
A_2	1	1	1	-1	-1	
B_1	1	1	$(-1)^p$	1	-1	
B_2	1	1	$(-1)^p$	-1	1	
$1 \leq \ell \leq n-1; E_\ell$	2	2	$2\cos \ell p\pi/n$	0	0	} $\alpha=-1$
$1 \leq \ell \leq n; E_{\ell\alpha}$	2	-2	$2\cos(2\ell-1)p\pi/2n$	0	0	
D_{2n}	E		A^p	$A^{2q}B$ $0 \leq q \leq n-1$	$A^{2q+1}B$ $0 \leq q \leq n-1$	$A^{2n}=B^2=E$ $BA=A^{2n-1}B$

$\mathcal{R}_2(D_{2n})$	$1 \leq p \leq 2n-1$					8n elements
	$1\epsilon_1$	$1\epsilon_2$	$2\epsilon_{4n/\text{hcf}(4n,p)}$	$2n\epsilon_2$ $0 \leq q \leq 2n-1$	$2n\epsilon_2$ $0 \leq q \leq 2n-1$	
	E	P^{2n}	P^{4n-p} P^P	$P^{2q}Q$	$P^{2q+1}Q$	$P^{4n}=Q^2=E$ $QP=P^{4n-1}Q$
A_1	1	1	1	1	1	} $\alpha=+1$
A_2	1	1	1	-1	-1	
B_1	1	1	$(-1)^P$	1	-1	
B_2	1	1	$(-1)^P$	-1	1	
$1 \leq \ell \leq n-1; E_\ell$	2	2	$2\cos \ell p\pi/n$	0	0	} $\alpha=-1$
$1 \leq \ell \leq n; E_{\ell\alpha}$	2	-2	$2\cos(2\ell-1)p\pi/2n$	0	0	
D_{2n}	E		A^P	$nA^{2q}B$ $0 \leq q \leq n-1$	$nA^{2q+1}B$ $0 \leq q \leq n-1$	$A^{2n}=B^2=E$ $BA=A^{2n-1}B$

	$1 \leq p \leq n-1$	$1 \leq p \leq 2n-1$	$1 \leq p \leq n-1$	$2\epsilon(2n-1)/\text{hcf}(2n-1, p)$	$(4n-2)\epsilon_4$ $0 \leq q \leq 2n-2$	$(4n-2)\epsilon_2$ $0 \leq q \leq 2n-2$	(16n-8) elements
$1\epsilon_1$	$2\epsilon_{4n-2}$	$2\epsilon(4n-2)/\text{hcf}(4n-2, p)$	$1 \leq p \leq n-1$	$2\epsilon(2n-1)/\text{hcf}(2n-1, p)$	$(4n-2)\epsilon_4$ $0 \leq q \leq 2n-2$	$(4n-2)\epsilon_2$ $0 \leq q \leq 2n-2$	$P^{4n-2} = Q^4 = E$
$1\epsilon_2$	$2\epsilon_{4n-2}$	$2\epsilon(4n-2)/\text{hcf}(4n-2, p)$	$1 \leq p \leq 2n-1$	$2\epsilon(2n-1)/\text{hcf}(2n-1, p)$	$(4n-2)\epsilon_4$ $0 \leq q \leq 2n-2$	$(4n-2)\epsilon_2$ $0 \leq q \leq 2n-2$	$QP = P^{4n-3} Q^3$
E	Q^2	Q^2	$P^{4n-2-2p} Q^2$	$P^{4n-1-2p} Q^2$	$P^{4n-2-2p}$	$P^{2q+1} Q^3$	$P^{2q+1} Q$
E	Q^2	Q^2	$P^{2p} Q^2$	P^{2p-1}	P^{2p}	$P^{2q+1} Q$	$P^{2q+1} Q$
A_1	1	1	1	1	1	1	1
A_2	1	1	1	1	1	-1	-1
B_1	1	1	1	-1	1	-1	-1
B_2	1	1	1	-1	1	1	1
$1 \leq \lambda \leq 2n-2; E_\lambda$	2	2	$2\cos\frac{2\lambda p\pi}{2n-1}$	$2\cos\frac{\lambda(2p-1)\pi}{2n-1}$	$2\cos\frac{2\lambda p\pi}{2n-1}$	0	0
E_α	2	-2	-2	0	2	0	0
$G_{\lambda\alpha}^+$	2	-2	$-2\cos\frac{4\lambda p\pi}{2n-1}$	$2i\sin\frac{2\lambda(2p-1)\pi}{2n-1}$	$2\cos\frac{4\lambda p\pi}{2n-1}$	0	0
$G_{\lambda\alpha}^-$	2	-2	$-2\cos\frac{4\lambda p\pi}{2n-1}$	$-2i\sin\frac{2\lambda(2p-1)\pi}{2n-1}$	$2\cos\frac{4\lambda p\pi}{2n-1}$	0	0
D_{4n-2}	E	A^{2p-1}	A^{2p-1}	A^{2p}	$(2n-1)A^{2q} B$	$(2n-1)A^{2q+1} B$	$A^{4n-2} = B^2 = E$
				$A^{4n-2-2p}$			$BA = A^{4n-3} B$

	$1 \leq p \leq 3n$	$1 \leq p \leq 2n-1$	$16n$ elements					
$\mathcal{R}_3(D_{4n})$	$1 \epsilon_1$	$2 \epsilon_2$	$2 \epsilon_{4n/hcf(4n, 2p-1)}$	$1 \epsilon_2$	$4n \epsilon_2$	$4n \epsilon_4$	$P^{8n} = Q^2 = E$	
	E	P^{4n}	$P^{4n-2p+1}$	P^{2p}	$P^{2q} Q$	$P^{2q+1} Q$		$QP = P^{4n-1} Q$
	A_1	1	1	1	1	1	$\alpha = +1$	
	A_2	1	1	1	-1	-1		
	B_1	1	-1	1	1	-1		
	B_2	1	-1	1	-1	1		
	$1 \leq \ell \leq 2n-1; E_\ell$	2	2	$2 \cos(2p-1)\ell\pi/2n$	$2 \cos \ell p\pi/n$	0	0	$\alpha = -1$
	$1 \leq \ell \leq 2n; G_{\ell\alpha} \left\{ \begin{matrix} G_{\ell\alpha}^+ \\ G_{\ell\alpha}^- \end{matrix} \right.$	2	-2	$2i \sin(2p-1)(2\ell-1)\pi/4n$	$2 \cos(2\ell-1)p\pi/2n$	0	0	
		2	-2	$-2i \sin(2p-1)(2\ell-1)\pi/4n$	$2 \cos(2\ell-1)p\pi/2n$	0	0	
	D_{4n}	E	A^{2p-1}	A^{2p}	$A^{2q} B$	$A^{2q+1} B$	$A^{4n} = B^2 = E$	
		$A^{4n-2p+1}$		$0 \leq q \leq 2n$	$0 \leq q \leq 2n$	$BA = A^{4n-1} B$		

$S_1(D_{2nh})$	$1c_1$	$1c_2$	$1c_2$	$1c_2$	$1c_2$	$1c_2$	$1c_2$	$1c_2$	$1p^{n-1}$ $2c_{2n}$	$1p^{n-1}$ $2c_{2n}$	$1p^{n-1}$ $2c_{2n}$	$1p^{2n}$ $4c_{4n}/\text{lcf}(4n, 2p-1)$	$1p^{2n-1}$ $2c_{2n}/\text{lcf}(2n, p)$
	x	p^{2n}	q^2	R^2	$Q^2 R^2$	$P^2 n Q^2$	$P^2 n R^2$	$P^2 n Q^2 R^2$	$p^{4n-2p} q^2$ $p^{2p} q^2$	$p^{4n-2p} R^2$ $p^{2p} R^2$	$p^{4n-2p} q^2$ $p^{2p} Q^2 R^2$	$p^{4n+1-2p} q^2$ $p^{2p-1} q^2$	p^{4n-2p} p^{2p}
A_{1g}	1	1	1	1	1	1	1	1	1	1	1	1	1
A_{2g}	1	1	1	1	1	1	1	1	1	1	1	1	1
B_{1g}	1	1	1	1	1	1	1	1	1	1	1	-1	1
B_{2g}	1	1	1	1	1	1	1	1	1	1	1	-1	1
A_{1u}	1	1	1	1	1	1	1	1	1	1	1	1	1
A_{2u}	1	1	1	1	1	1	1	1	1	1	1	1	1
B_{1u}	1	1	1	1	1	1	1	1	1	1	1	-1	1
B_{2u}	1	1	1	1	1	1	1	1	1	1	1	-1	1
$1s2n-1; E_{1g}$	2	2	2	2	2	2	2	2	$2\cos 2tp/n$	$2\cos 2tp/n$	$2\cos 2tp/n$	$2\cos(2p-1)t/n$	$2\cos 2tp/n$
$1s2n-1; E_{1u}$	2	2	2	2	2	2	2	2	$2\cos 2tp/n$	$2\cos 2tp/n$	$2\cos 2tp/n$	$2\cos(2p-1)t/n$	$2\cos 2tp/n$
$1s2n; E_{2g}$	2	-2	2	2	2	-2	-2	-2	$2\cos(2t-1)pn/n$	$2\cos(2t-1)pn/n$	$2\cos(2t-1)pn/n$	$2\cos(2t-1)(2p-1)t/2n$	$2\cos(2t-1)pn/n$
E_{1g}	2	2	-2	2	-2	2	-2	-2	-2	2	-2	2	2
E_{2g}	2	2	-2	2	-2	2	-2	-2	-2	2	-2	-2	2
$1s2n-1; G_{1g}$	G_{1g}^+	2	2	-2	2	-2	2	-2	$-2\cos 2tp/n$	$2\cos 2tp/n$	$-2\cos 2tp/n$	$2\cos(2p-1)t/n$	$2\cos 2tp/n$
	G_{1g}^-	2	2	-2	2	-2	2	-2	$-2\cos 2tp/n$	$2\cos 2tp/n$	$-2\cos 2tp/n$	$2\cos(2p-1)t/n$	$2\cos 2tp/n$
E_{1y}	2	2	2	-2	-2	2	-2	-2	2	-2	-2	0	2
E_{2y}	2	2	2	-2	-2	2	-2	-2	2	-2	-2	0	2
n even; G_y	G_y^+	2	2	2	-2	-2	2	-2	$2(-1)^p$	$2(-1)^{p+1}$	$2(-1)^{p+1}$	0	$2(-1)^p$
	G_y^-	2	2	2	-2	-2	2	-2	$2(-1)^p$	$2(-1)^{p+1}$	$2(-1)^{p+1}$	0	$2(-1)^p$
$1s2n(n-1); G_{1y}$	4	4	4	-4	-4	4	-4	-4	$4\cos 2tp/n$	$-4\cos 2tp/n$	$-4\cos 2tp/n$	0	$4\cos 2tp/n$
$1s2n; G_{1u}$	G_{1u}^+	2	-2	-2	2	-2	2	2	$-2\cos(2t-1)pn/n$	$2\cos(2t-1)pn/n$	$-2\cos(2t-1)pn/n$	$2\cos(2t-1)(2p-1)t/2n$	$2\cos(2t-1)pn/n$
	G_{1u}^-	2	-2	-2	2	-2	2	2	$-2\cos(2t-1)pn/n$	$2\cos(2t-1)pn/n$	$-2\cos(2t-1)pn/n$	$2\cos(2t-1)(2p-1)t/2n$	$2\cos(2t-1)pn/n$
n odd; G_{1y}	G_{1y}^+	2	-2	2	-2	-2	2	2	$2(-1)^p$	$2(-1)^{p+1}$	$2(-1)^{p+1}$	0	$2(-1)^p$
	G_{1y}^-	2	-2	2	-2	-2	2	2	$2(-1)^p$	$2(-1)^{p+1}$	$2(-1)^{p+1}$	0	$2(-1)^p$
$1s2n; G_{2y}$	G_{2y}^+	4	-4	4	-4	-4	4	4	$4\cos(2t-1)pn/n$	$-4\cos(2t-1)pn/n$	$-4\cos(2t-1)pn/n$	0	$4\cos(2t-1)pn/n$
	G_{2y}^-	2	2	-2	-2	2	-2	2	-2	-2	2	0	2
n even; E_{1y}	E_{1y}^+	2	2	-2	-2	2	-2	2	$2(-1)^{p+1}$	$2(-1)^{p+1}$	$2(-1)^p$	0	$2(-1)^p$
	E_{1y}^-	2	2	-2	-2	2	-2	2	$2(-1)^{p+1}$	$2(-1)^{p+1}$	$2(-1)^p$	0	$2(-1)^p$
$1s2n(n-1); G_{2y}$	4	4	-4	-4	4	-4	-4	-4	$-4\cos 2tp/n$	$-4\cos 2tp/n$	$4\cos 2tp/n$	0	$4\cos 2tp/n$
n odd; E_{1uy}	2	-2	-2	-2	2	2	-2	-2	$2(-1)^{p+1}$	$2(-1)^{p+1}$	$2(-1)^p$	0	$2(-1)^p$
n odd; E_{2uy}	2	-2	-2	-2	2	2	-2	-2	$2(-1)^{p+1}$	$2(-1)^{p+1}$	$2(-1)^p$	0	$2(-1)^p$
$1s2n; G_{2uy}$	4	-4	-4	-4	4	4	-4	-4	$-4\cos(2t-1)pn/n$	$-4\cos(2t-1)pn/n$	$4\cos(2t-1)pn/n$	0	$4\cos(2t-1)pn/n$

continues.....

$1 \leq p \leq n$	$1 \leq p \leq 2n$	$0 \leq p \leq 2n-1$									6n elements	
$4^c \text{An/hcf}(4n, 2p-1)$	$4^c \text{An/hcf}(4n, 2p-1)$	$4^c \text{An/hcf}(2n-3, p)$	$4n_4$	$4n_4$	$4n_4$	$4n_4$	$4n_4$	$4n_4$	$4n_4$	$4n_2$	$4n_2$	
$p^{4n+1-2p} Q^2 R^2$	$p^{4n+1-2p} Q^2 R^3$	$p^{4n-2p} Q^2 R^3$	$0 < q < 2n-1$	$0 < q < 2n-1$	$1 < q < 2n$	$1 < q < 2n$	$0 < q < n-1$	$0 < q < n-1$	$1 < q < n$	$1 < q < n$	$1 < q < n$	$p^{4n-4} R^4 - E$
$p^{2p-1} Q^2 R^2$	$p^{4n+1-2p} Q^2 R$	$p^{4n-2p} Q^2 R$	$p^{2q} Q^3$	$p^{2q} Q^3 R^2$	$p^{2q-1} Q^3 R^2$	$p^{2q-1} Q^3 R^2$	$p^{4q+2} Q^3 R$	$p^{4q+2} Q^3 R^3$	$p^{4q-3} Q^3 R^3$	$p^{4q-3} Q^3 R^3$	$p^{4q-3} Q^3 R^3$	$Q^4 - p^{4n-1} Q; BQ^4 R^3$
$p^{4n+1-2p} Q^2$	$p^{2p-1} R^3$	$p^{2p} R^3$	$p^{2q} Q$	$p^{2q} Q R^2$	$p^{2q-1} Q$	$p^{2q-1} Q^3$	$p^{4q} Q^3 R^3$	$p^{4q} Q^3 R^3$	$p^{4q-1} Q^3 R^3$	$p^{4q-1} Q^3 R^3$	$p^{4q-1} Q^3 R^3$	$RA - R^3 P$
$p^{2p-1} Q^2$	$p^{2p-1} R$	$p^{2p} R$	$p^{2q} Q$	$p^{2q} Q R^2$	$p^{2q-1} Q$	$p^{2q-1} Q^3$	$p^{4q} Q^3 R^3$	$p^{4q} Q^3 R^3$	$p^{4q-1} Q^3 R^3$	$p^{4q-1} Q^3 R^3$	$p^{4q-1} Q^3 R^3$	
1	1	1	1	1	1	1	1	1	1	1	1	
1	1	1	-1	-1	-1	-1	-1	-1	-1	-1	-1	
-1	$(-1)^{n-1}$	$(-1)^n$	1	1	-1	-1	1	1	-1	-1	-1	
-1	$(-1)^{n-1}$	$(-1)^n$	-1	-1	1	1	-1	-1	1	1	1	
1	-1	-1	-1	-1	-1	-1	1	1	1	1	1	
1	-1	-1	1	1	1	1	-1	-1	-1	-1	-1	$\alpha=0; \beta=0; \gamma=0$
-1	$(-1)^n$	$(-1)^{n-1}$	-1	-1	1	1	1	1	1	-1	-1	
-1	$(-1)^n$	$(-1)^{n-1}$	1	1	-1	-1	-1	-1	-1	1	1	
$2 \cos(2p-1)\pi/n$	$(-1)^k 2 \cos(2p-1)\pi/n$	$(-1)^k 2 \cos 2kp\pi/n$	0	0	0	0	0	0	0	0	0	
$2i \cos(2p-1)\pi/n$	$(-1)^{k+1} 2i \cos(2p-1)\pi/n$	$(-1)^{k+1} 2i \cos 2kp\pi/n$	0	0	0	0	0	0	0	0	0	
$2 \cos(2k-1)(2p-1)\pi/2n$	$(-1)^k 2 \cos(2k-1)(2p-1)\pi/2n$	$(-1)^k 2 \cos(2k-1)kp\pi/n$	0	0	0	0	0	0	0	0	0	$\alpha=-1; \beta=0; \gamma=0$
-2	0	0	0	0	0	0	0	0	0	0	0	
2	0	0	0	0	0	0	0	0	0	0	0	
$-2 \cos(2p-1)\pi/n$	$2i \sin(2p-1)\pi/n$	$2i \sin 2kp\pi/n$	0	0	0	0	0	0	0	0	0	$\alpha=0; \beta=-1; \gamma=0$
$-2i \cos(2p-1)\pi/n$	$-2i \sin(2p-1)\pi/n$	$-2i \sin 2kp\pi/n$	0	0	0	0	0	0	0	0	0	
0	0	0	2	-2	0	0	0	0	0	0	0	
0	0	0	-2	2	0	0	0	0	0	0	0	
0	0	0	0	0	0	0	2i	-2i	0	0	0	$\alpha=0; \beta=0; \gamma=-1$
0	0	0	0	0	0	0	-2i	2i	0	0	0	
$-2 \cos(2k-1)(2p-1)\pi/2n$	$2i \sin(2k-1)(2p-1)\pi/2n$	$2i \sin(2k-1)kp\pi/n$	0	0	0	0	0	0	0	0	0	$\alpha=-1; \beta=-1; \gamma=0$
$-2i \cos(2k-1)(2p-1)\pi/2n$	$-2i \sin(2k-1)(2p-1)\pi/2n$	$-2i \sin(2k-1)kp\pi/n$	0	0	0	0	0	0	0	0	0	
0	0	0	0	0	0	0	2i	-2i	0	0	0	
0	0	0	0	0	0	0	-2i	2i	0	0	0	$\alpha=-1; \beta=0; \gamma=-1$
0	0	0	0	0	0	2i	-2i	0	0	0	0	
0	0	0	0	0	-2i	2i	0	0	0	0	0	
0	0	0	0	0	0	0	0	0	2	-2	-2	$\alpha=0; \beta=-1; \gamma=-1$
0	0	0	0	0	0	0	0	0	-2	2	2	
0	0	0	0	0	0	0	0	0	0	0	0	
0	0	0	0	0	0	0	0	0	0	2	-2	
0	0	0	0	0	0	0	0	0	-2	2	2	$\alpha=-1; \beta=-1; \gamma=-1$
0	0	0	0	0	0	0	0	0	0	0	0	

$A^{2p-1}C$ $A^{2p}C$ $A^{2n}B$ $A^{2q-1}B$ $A^{4q}C$ $A^{4q-2}BC$ $A^{4q-2}DC$ $A^{4q-1}AC$ $A^{2n}B^2 - C^2 - E$
 $0 < q < n-1$ $1 < q < n$ $0 < q < (n-1)$ $1 < q < n$ $1 < q < n$ $1 < q < n$ $1 < q < n$ $1 < q < n$ $2A - A^{2n-1}B$
 $CA - AC; CB - BC$

	$1\epsilon_1$	$1\epsilon_2$	$6\epsilon_4$	$4\epsilon_6$	$4\epsilon_6$	$4\epsilon_3$	$4\epsilon_3$	24 elements	
				PR	P^3QR^2	R^2	R	$P^4=Q^4=R^3=E$	
		P, P^3	QR	P^3R^2	PR^2	P^2QR		$P^2=Q^2$	
		Q, P^2Q	PQR	P^2QR^2	QR^2	P^3QR		$QP=P^3Q; RP=QR$	
$\mathcal{R}(T)$	E	P^2	PQ, P^3Q	P^2R	P^2R^2	PQR^2	P^3R	$RQ=PQR$	
A	1	1	1	1	1	1	1		
E	E^+	1	1	1	ω	ω^*	ω^*	ω	} $\alpha=+1$
	E^-	1	1	1	ω^*	ω	ω	ω^*	
T	3	3	-1	0	0	0	0		
$E_{\frac{1}{2}}$	2	-2	0	1	1	-1	-1		} $\alpha=-1$
$G_{\frac{3}{2}}^+$	2	-2	0	ω	ω^*	$-\omega^*$	$-\omega$		
$G_{\frac{3}{2}}^-$	2	-2	0	ω^*	ω	$-\omega$	$-\omega^*$		
T	E	A	AC	C^2	C	$A^2=B^2=C^3=E$			
		B	BC	AC^2		AB=BA			
		AB	ABC	BC^2		CA=BC			
				ABC^2		CB=ABC			

$$(\omega=e^{2\pi i/3})$$

$R_I(T_h)$ is the direct product group $R(T) \times \{E, I\}$

$R_2(T_h)$	$1\epsilon_1$	$1\epsilon_2$	$6\epsilon_4$	$4\epsilon_3$	$4\epsilon_3$	$4\epsilon_6$	$4\epsilon_6$	$1\epsilon_4$	$1\epsilon_4$	$6\epsilon_2$	$4\epsilon_{12}$	$4\epsilon_{12}$	$4\epsilon_{12}$	$4\epsilon_{12}$	48 elements	
											P^3QT					
											P^2QT				$P^4=Q^4=R^3=T^4=E$	
				P^2QR	PR^2	PQR	P^2QR^2			P^3T	P^2QRT	P^3R^2T	PR^2T	QRT	$P^2=Q^2=T^2$	
			PQ, P^3Q	P^3QR	QR^2	P^2R	P^2R^2			PQT	P^3QRT	P^2QR^2T	QR^2T	$PQRT$	$QP=P^3Q; RP=QR$	
			Q, P^2Q	P^3R	PQR^2	QR	P^3R^2			QT	P^3RT	P^3QR^2T	PQR^2T	PRT	$RQ=PQR; TR=RT$	
	E	P^2	P, P^3	R	R^2	PR	P^3QR^2	T	P^2T	PT	RT	P^2R^2T	R^2T	P^2RT	$TP=PT; TQ=QT$	
E_g	A_g	1	1	1	1	1	1	1	1	1	1	1	1	1	} $\alpha=+1$	
	E_g^+	1	1	1	ω	ω^*	ω	ω^*	1	1	1	ω	ω^*	ω		
	E_g^-	1	1	1	ω^*	ω	ω^*	ω	1	1	1	ω^*	ω	ω^*		
T_g	3	3	-1	0	0	0	0	3	3	-1	0	0	0			
E_u	A_u	1	1	1	1	1	1	-1	-1	-1	-1	-1	-1	-1		
	E_u^+	1	1	1	ω	ω^*	ω	ω^*	-1	-1	-1	$-\omega$	$-\omega^*$	$-\omega$		
	E_u^-	1	1	1	ω^*	ω	ω^*	ω	-1	-1	-1	$-\omega^*$	$-\omega$	$-\omega^*$		
	T_u	3	3	-1	0	0	0	-3	-3	1	0	0	0			
G_a	C_a^+	2	-2	0	-1	-1	1	1	-2i	2i	0	i	-i	-i	} $\alpha=-1$	
	C_a^-	2	-2	0	-1	-1	1	1	2i	-2i	0	-i	i	-i		
G'_a	C'_a^+	2	-2	0	$-\omega$	$-\omega^*$	ω	ω^*	-2i	2i	0	$i\omega$	$-i\omega^*$	$i\omega^*$		-i\omega
	C'_a^-	2	-2	0	$-\omega^*$	$-\omega$	ω^*	ω	2i	-2i	0	$-i\omega^*$	$i\omega$	$-i\omega$		$i\omega^*$
G''_a	C''_a^+	2	-2	0	$-\omega^*$	$-\omega$	ω^*	ω	-2i	2i	0	$i\omega^*$	$-i\omega$	$i\omega$		$-i\omega^*$
	C''_a^-	2	-2	0	$-\omega$	$-\omega^*$	ω	ω^*	2i	-2i	0	$-i\omega$	$i\omega^*$	$-i\omega^*$		$i\omega$
T_h	E	A	C	C^2	AC			I		AI	CI	C^2I	ACI	AC^2I	ACI	$A^2=B^2=C^3=I^2=E$
		B		AC^2	BC					BI		AC^2I	BCI		$BA=AB; CA=BC$	
		AB		BC^2	ABC					ABI		BC^2I	$ABCI$		$CB=ABC; IA=AI$	
				ABC^2								ABC^2I			$IB=BI; IC=CI$	

$\omega = \exp(2\pi i/3)$

	1ε1	1ε2	6ε4	8ε6	8ε3	12ε4	6ε8	6ε8	48 elements
						S, P ² S			P ⁴ =Q ⁴ =R ³ =S ⁴ =E
						PQS, P ³ QS			P ² =Q ² =S ²
						R ² S, P ² R ² S			QP=P ³ Q; FP=QR
						RS, P ² RS	PS, P ² QS	QS, P ³ S	RQ=P ³ QR; SP=P ² QS
						PR ² , P ² QR	QR, P ³ R ²		SQ=P ³ S; SR=R ² S
						QR ² , PQR	P ² R, P ² R ²		
						P, P ³	Q, P ² Q		
						PR ² , P ² QR	P ³ QR, P ² QR ²	P ² QS, P ³ QRS	
						QR ² , PQR	P ³ R, P ³ QR ²	P ² QR ² S, P ³ QR ² S	
$\mathcal{N}_1(0)$	E	P ²	PQ, P ³ Q	P ³ R, P ³ QR ²	P ³ QR, P ² QR ²	QRS, P ² QRS	P ² QS, P ³ QRS	P ² QR ² S, P ³ QR ² S	
A ₁	1	1	1	1	1	1	1	1	} α=+1
A ₂	1	1	1	1	1	-1	-1	-1	
E	2	2	2	-1	-1	0	0	0	
T ₁	3	3	-1	0	0	-1	1	1	
T ₂	3	3	-1	0	0	1	-1	-1	
E ₁	2	-2	0	1	-1	0	√2	-√2	} α=-1
E ₂	2	-2	0	1	-1	0	-√2	√2	
G ₂	4	-4	0	-1	1	0	0	0	
O	E	A	AC ²	AC ²	C ² , C	D	AD	BD	A ² =B ² =C ³ =D ² =E
		B	BC ² , ABC	AC, ABC ²	AC, ABC ²	ABD	BC ² D, ABC ² D	ACD, ABCD	BA=AB; CA=BC
		AB		BC	BC	C ² D			CB=ABC; DA=BD
						CD			DB=AD; DC=C ² D
						AC ² D			
						BCD			

	$1\epsilon_1$	$1\epsilon_2$	$6\epsilon_4$	$8\epsilon_6$	$8\epsilon_3$	$12\epsilon_2$	$6\epsilon_4$	$6\epsilon_4$	48 elements
						$S;P^2S$	PS	QS	$P^4=Q^4=R^3=S^2=E$
						$PQS;P^3QS$	P^2QS	P^3S	$P^2=Q^2$
						$R^2S;RS$	$PQRS$	FRS	$QP=P^3Q;RP=QR$
						PR,P^3QR^2	R^2,R		$RQ=PQR;SP=P^2QS$
						QR,P^3R^2	PR^2,P^2QR	P^2QR^2S	$SQ=P^3S;SR=R^2S$
						P,P^3	QR,P^2QR		
						Q,P^2Q	QR,P^2QR^2	QR^2S	
						P^2R,P^2R^2	PQR^2,P^3R	P^3QRS	
$P_2(0)$	E	P^2	PQ,P^3Q	P^2R,P^2R^2	PQR^2,P^3R	$P^2RS;P^2R^2S$	P^3RS		
A_1	1	1	1	1	1	1	1	1	} $\alpha=+1$
A_2	1	1	1	1	-1	-1	-1	-1	
E	2	2	-1	-1	0	0	0	0	} $\alpha=-1$
T_1	3	3	0	0	-1	1	1	1	
T_2	3	3	-1	0	1	-1	-1	-1	
G_2^+	4	-4	0	-1	1	0	0	0	
G_1^+	2	-2	0	1	-1	0	$i\sqrt{2}$	$-i\sqrt{2}$	
G_1^-	2	-2	0	1	-1	0	$-i\sqrt{2}$	$i\sqrt{2}$	
O	E	A	AC	C^2,C	D	AD	BD	$A^2=B^2=C^3=D^2=E$	
	B	BC	AC^2	ABD	$BA=AB; CA=BC$				
	AB	ABC	BC^2	$C^2D; CD$	$ABCD$	ACD	$CB=ABC; DA=BD$		
			ABC^2	AC^2D	BCD	BC^2D	$DB=AD; DC=C^2D$		



	1e1	1e2	1e2	1e2	6e4	8e6	8e3	24e4	12e8	12e8	6e4	8e6	8e6
$\mathcal{P}_1(O_h)$	E	P2	S2	P2S2	P0, P3Q	P2R, P2R2	PQR2, P3R	RS, RS3	P3QR5, P2QR2S3	P3QR5, P2QR2S3	PS2, P3QS2	QRS2, P3RS2	P2RS2, P3RS2
A1R	1	1	1	1	1	1	1	1	1	1	1	1	1
A2B	1	1	1	1	-1	1	1	-1	-1	1	1	1	1
Eg	2	2	2	2	0	-1	0	0	0	0	2	-1	-1
T1B	3	3	3	3	-1	0	0	-1	1	1	-1	0	0
T2B	3	3	3	3	-1	0	0	1	-1	-1	-1	0	0
A1u	1	1	1	1	1	1	1	1	1	1	1	1	1
A2u	1	1	1	1	1	1	1	-1	-1	-1	1	1	1
Eu	2	2	2	2	2	-1	-1	0	0	0	2	-1	-1
T1u	3	3	3	3	-1	0	0	-1	1	1	-1	0	0
T2u	3	3	3	3	-1	0	0	1	-1	-1	-1	0	0
Gg	4	-4	4	-4	0	2	-2	0	0	0	0	2	-2
$K_a \{ K_a \}$	4	-4	4	-4	0	-1	1	0	0	0	0	-1	1
	4	-4	4	-4	0	-1	1	0	0	0	0	-1	1
$G_B \{ G_B \}$	2	2	-2	-2	2	2	2	0	0	0	-2	-2	-2
	2	2	-2	-2	2	-1	-1	0	0	0	-2	-2	-2
I _B	6	6	-6	-6	-2	0	0	0	0	0	2	0	0
	2	-2	-2	2	0	1	-1	0	$\sqrt{2}$	$-\sqrt{2}$	0	-1	1
E _{gB}	2	-2	-2	2	0	1	-1	0	$\sqrt{2}$	$-\sqrt{2}$	0	-1	1
	2	-2	-2	2	0	1	-1	0	$-\sqrt{2}$	$\sqrt{2}$	0	-1	1
E _{gU}	2	-2	-2	2	0	1	-1	0	$-\sqrt{2}$	$\sqrt{2}$	0	-1	1
	2	-2	-2	2	0	1	-1	0	$\sqrt{2}$	$-\sqrt{2}$	0	-1	1
G _{gB}	4	-4	-4	4	0	-1	1	0	0	0	0	1	-1
	4	-4	-4	4	0	-1	1	0	0	0	0	1	-1
G _{gU}	4	-4	-4	4	0	-1	1	0	0	0	0	1	-1
O _h	E	A	AC	C ² , C	D	AD	BD	BD	BD	BD	BD	BD	BD
		B	BC	AC ²	ABD	ABCD	ACD	ACD	ACD	ACD	ACD	ACD	ACD
		AB	ABC	ABC ²	AC ² D	BC ² D	ABC ² D	ABC ² D	ABC ² D	ABC ² D	ABC ² D	ABC ² D	ABC ² D

continues.....

2ε ₂	2ε ₂	12ε ₄	8ε ₆	8ε ₆	8ε ₆	8ε ₆	24ε ₄	12ε ₈	12ε ₈	192 elements
1	1	1	1	1	1	1	1	1	1	P ⁴ =Q ⁴ =R ³ =S ⁴ =T ² =E P ² =Q ²
1	1	1	1	1	1	1	1	1	1	
2	2	2	-1	-1	-1	0	0	0	0	
3	3	-1	0	0	0	-1	1	1	1	
3	3	-1	0	0	0	1	1	-1	-1	
-1	-1	-1	-1	-1	-1	-1	-1	-1	-1	
-1	-1	-1	-1	-1	-1	1	1	1	1	
-2	-2	-2	1	1	1	0	0	0	0	
-3	-3	1	0	0	0	1	1	-1	-1	
-3	-3	1	0	0	0	-1	1	1	1	
0	0	0	0	0	0	0	0	0	0	
0	0	0	-i√3	i√3	i√3	0	0	0	0	
0	0	0	i√3	-i√3	-i√3	0	0	0	0	
0	0	0	0	0	0	0	0	0	0	
0	0	0	-i√3	i√3	-i√3	0	0	0	0	
0	0	0	i√3	-i√3	i√3	0	0	0	0	
0	0	0	0	0	0	0	0	0	0	
2	-2	0	1	1	-1	0	0	√2	√2	
-2	2	0	-1	-1	1	0	0	√2	-√2	
2	-2	0	1	1	-1	0	0	-√2	√2	
-2	2	0	-1	-1	1	0	0	-√2	-√2	
4	-4	0	-1	1	1	0	0	0	0	
-4	4	0	1	-1	-1	0	0	0	0	
I		AI BI ABI	ACI BCI ABC1	C ² I AC ² I BC ² I ABC ² I	CI	DI ABDI C ² DI AC ² DI BCDI CDI	ADI ABCDI BC ² DI	BDI ACDI ABC ² DI		A ² =B ² C ² =D ² =I ² =E EA=AB; CA=BC; CB=ABC DA=BD; DB=AD; DC=C ² D; IA=AI; IB=BI; IC=CI; ID=DI.

α=+1; β=+1

α=-1; β=+1

α=+1; β=-1

α=-1; β=-1

$R_2(0_h)$

	$1e_1, 1e_2$	$1e_2$	$1e_2$	$6e_4$	$8e_6$	$8e_3$	$24e_2$	$12e_8$	$12e_8$	$6e_4$	$8e_6$	$8e_6$
A_{1g}	1	1	1	1	1	1	1	1	1	1	1	1
A_{2g}	1	1	1	1	1	1	-1	-1	-1	1	1	1
E_g	2	2	2	2	-1	-1	0	0	0	2	-1	-1
T_{1g}	3	3	3	-1	0	0	-1	1	1	-1	0	0
T_{2g}	3	3	3	-1	0	0	1	-1	-1	-1	0	0
A_{1u}	1	1	1	1	1	1	1	1	1	1	1	1
A_{2u}	1	1	1	1	1	1	-1	-1	-1	1	1	1
E_u	2	2	2	2	-1	-1	0	0	0	2	-1	-1
T_{1u}	3	3	3	-1	0	0	-1	1	1	-1	0	0
T_{2u}	3	3	3	-1	0	0	1	-1	-1	-1	0	0
G'_{ag}	4	-4	4	0	-1	1	0	0	0	0	-1	1
G'_{au}	4	-4	4	0	-1	1	0	0	0	0	-1	1
$G''_{ag} \begin{pmatrix} C''_{ag} \\ C''_{ag} \end{pmatrix}$	2	-2	2	0	1	-1	0	$i\sqrt{2}$	$-i\sqrt{2}$	0	1	-1
$G''_{ag} \begin{pmatrix} C''_{ag} \\ C''_{ag} \end{pmatrix}$	2	-2	2	0	1	-1	0	$-i\sqrt{2}$	$i\sqrt{2}$	0	1	-1
$G''_{au} \begin{pmatrix} C''_{au} \\ C''_{au} \end{pmatrix}$	2	-2	2	0	1	-1	0	$i\sqrt{2}$	$-i\sqrt{2}$	0	1	-1
$G''_{au} \begin{pmatrix} C''_{au} \\ C''_{au} \end{pmatrix}$	2	-2	2	0	1	-1	0	$-i\sqrt{2}$	$i\sqrt{2}$	0	1	-1
E_B	2	2	-2	2	2	2	0	0	0	2	-2	-2
E_B	2	2	-2	2	-1	-1	0	0	0	2	1	1
E_B	2	2	-2	2	-1	-1	0	0	0	2	1	1
I_B	6	6	-6	-2	0	0	0	0	0	-2	0	0
G_{ag}	4	-4	4	0	2	-2	0	0	0	0	-2	2
G_{ag}	4	-4	4	0	-1	1	0	0	0	0	1	-1
G_{au}	4	-4	4	0	-1	1	0	0	0	0	1	-1

	E	A	AC	C ² , C	D	AD	BD
A_{1g}							
A_{2g}							
E_g							
T_{1g}							
T_{2g}							
A_{1u}							
A_{2u}							
E_u							
T_{1u}							
T_{2u}							
G'_{ag}							
G'_{au}							
$G''_{ag} \begin{pmatrix} C''_{ag} \\ C''_{ag} \end{pmatrix}$							
$G''_{ag} \begin{pmatrix} C''_{ag} \\ C''_{ag} \end{pmatrix}$							
$G''_{au} \begin{pmatrix} C''_{au} \\ C''_{au} \end{pmatrix}$							
$G''_{au} \begin{pmatrix} C''_{au} \\ C''_{au} \end{pmatrix}$							
E_B							
E_B							
E_B							
I_B							
G_{ag}							
G_{ag}							
G_{au}							

continues.....

2ε ₄	2ε ₄	12ε ₄	8ε ₁₂	8ε ₁₂	8ε ₁₂	8ε ₁₂	8ε ₁₂	24ε ₂	12ε ₈	12ε ₈	192 elements
								ST;ST ³	PST	QST	P ⁴ =Q ⁴ -R ³ =S ² -T ⁴ =E
								POST;POST ³	P ² QST	P ³ ST	P ² =Q ²
								R ² ST;R ² ST ³	PQRST	PRST	QP=P ³ Q;RP=QR;RQ=PQR;
								PR ² ST;PR ² ST ³	P ³ RST	P ³ QRST	SP=P ² QS;SQ=P ³ S;SR=R ² S;
								QRST;QRST ³	QR ² ST	P ² QRST	TP=PT;TQ=QT;TR=RT;
								P ² RST;P ² RST ³	P ³ QR ² ST	P ² QRST	TS=ST ³
								P ² ST;P ² ST ³	PST ³	QST ³	
								P ³ QST;P ³ QST ³	P ² QST ³	P ³ ST ³	
								P ² R ² ST;P ² R ² ST ³	P ² QRST ³	PRST ³	
								P ³ R ² ST;P ³ R ² ST ³	P ³ RST ³	P ³ QRST ³	
								P ² QRST;P ² QRST ³	QR ² ST ³	PQR ² ST ³	
								P ³ QRST;P ³ QRST ³	P ³ QR ² ST ³	P ² QRST ³	
T, T ³	P ² T, P ² T ³	PQT, P ³ QT	P ² RT, P ² RT ³	P ² R ² T, P ² R ² T ³	P ³ RT, P ³ RT ³	P ² T, P ² T ³	R ² T ³ , RT	P ³ QST;P ³ QST ³	P ² QST ³	P ³ ST ³	
								P ² R ² ST;P ² R ² ST ³	P ² QRST ³	PRST ³	
1	1	1	1	1	1	1	1	1	1	1	α=+1; β=+1
1	1	1	1	1	1	1	1	-1	-1	-1	
2	2	2	-1	-1	-1	-1	-1	0	0	0	
3	3	-1	0	0	0	0	0	-1	1	1	
3	-1	-1	0	0	0	0	0	1	-1	-1	
-1	-1	-1	-1	-1	-1	-1	-1	-1	-1	-1	
-1	-1	-1	-1	-1	-1	-1	-1	1	1	1	
-2	-2	1	1	1	1	1	1	0	0	0	
-3	-3	1	0	0	0	0	0	1	-1	-1	
-3	-3	1	0	0	0	0	0	-1	1	1	
4	-4	0	-1	-1	-1	-1	-1	0	0	0	
-4	4	0	1	1	1	1	1	0	0	0	
2	-2	0	1	1	1	1	1	0	i√2	-i√2	
2	-2	0	1	1	1	1	1	0	-i√2	i√2	
-2	2	0	-1	-1	-1	-1	-1	0	-i√2	i√2	
-2	2	0	-1	-1	-1	-1	-1	0	i√2	-i√2	
0	0	0	0	0	0	0	0	0	0	0	
0	0	0	-√3	-√3	-√3	-√3	-√3	0	0	0	
0	0	0	√3	√3	√3	√3	√3	0	0	0	
0	0	0	0	0	0	0	0	0	0	0	
0	0	0	0	0	0	0	0	0	0	0	
0	0	0	-√3	-√3	-√3	-√3	-√3	0	0	0	
0	0	0	√3	√3	√3	√3	√3	0	0	0	
0	0	0	-√3	-√3	-√3	-√3	-√3	0	0	0	
0	0	0	√3	√3	√3	√3	√3	0	0	0	
I	AI	ACI	C ² I	CI	DI	ADI	BDI	A ² =B ² =C ³ =D ² =I ² =E			
	BI	BCI	AC ² I	AE ² I	ABDI	ABCI	BA=AB; CA=BC; CB=ABC;				
	ABI	ABCI	BC ² I	BC ² I	C ³ DI	ABCDI	ACDI	DA=BD; DB=AD; DC=C ² D;			
			ABC ² I	ABC ² I	AC ² DI	BC ² DI	ABC ² DI	IA=AI; IB=BI; IC=CI;			
					BCDI	BC ² DI	ABC ² DI	ID=DI			

	$1c_1$	$1c_2$	$1c_2$	$1c_2$	$6c_4$	$8c_6$	$8c_3$	$24c_4$	$12c_8$	$12c_8$	$6c_4$	$8c_6$	$8c_6$	$2c_4$	$2c_4$
								S, S^3	PS	QS^3					
								PQS, PQS^3	P^2QS	P^3S^3					
								R^2S, R^2S^3	$PQRS$	PRS^3					
								Pk^2S, PR^2S^3	P^3RS	P^3QRS^3					
								QRS, QRS^3	QR^2S	PQR^2S					
								P^2RS, P^2RS^3	P^3QR^2S	$P^2QR^2S^3$					
								P^2S, P^2S^3	PS^3	QS					
								P^3QS, P^3QS^3	P^2QS^3	P^3S					
						PR, P^3QR^2	R^2, R	$P^2R^2S, P^2R^2S^3$	$PQRS^3$	PRS		$FRS^2, P^3QR^2S^2$	R^2S^2, RS^2		
					P, P^3	QR, P^3R^2	PR^2, P^2QR	$P^3R^2S, P^3R^2S^3$	P^3RS^3	P^3QRS	PS^2, P^3S^2	$QRS^2, P^3R^2S^2$	PR^2S^2, P^2QRS^2		
					Q, P^2Q	PQR, P^2QR^2	QR^2, P^3QR	P^2QRS, P^2QRS^3	QR^2S^3	PQR^2S	QS^2, P^2QS^2	$PQRS^2, P^2Qk^2S^2$	QR^2S^2, P^3QRS^2		
$3(O_h)$	E	P^2	S^2	P^2S^2	PQ, P^3Q	P^2R, P^2R^2	PQR^2, P^3R	RS, RS^3	$P^3QR^2S^3$	P^2QR^2S	PQS^2, P^3QS^2	$P^2RS^2, P^2R^2S^2$	PQR^2S^2, P^3RS^2	T, S^2T	P^2T, P^2S^2T
A_{1g}	1	1	1	1	1	1	1	1	1	1	1	1	1	1	1
A_{2g}	1	1	1	1	1	1	1	-1	-1	-1	1	1	1	1	1
E_g	2	2	2	2	2	-1	-1	0	0	0	2	-1	-1	2	2
T_{1g}	3	3	3	3	-1	0	0	-1	1	1	-1	0	0	3	3
T_{2g}	3	3	3	3	-1	0	0	1	-1	-1	-1	0	0	3	3
A_{1u}	1	1	1	1	1	1	1	1	1	1	1	1	1	-1	-1
A_{2u}	1	1	1	1	1	1	1	-1	-1	-1	1	1	1	-1	-1
E_u	2	2	2	2	2	-1	-1	0	0	0	2	-1	-1	-2	-2
T_{1u}	3	3	3	3	-1	0	0	-1	1	1	-1	0	0	-3	-3
T_{2u}	3	3	3	3	-1	0	0	1	-1	-1	-1	0	0	-3	-3
G_{ag}^+	4	-4	4	-4	0	-1	1	0	0	0	0	-1	1	4	-4
G_{au}^+	4	-4	4	-4	0	-1	1	0	0	0	0	-1	1	-4	4
G_{ag}^{u+}	2	-2	2	-2	0	1	-1	0	$i\sqrt{2}$	$-i\sqrt{2}$	0	1	-1	2	-2
G_{ag}^{u-}	2	-2	2	-2	0	1	-1	0	$-i\sqrt{2}$	$i\sqrt{2}$	0	1	-1	2	-2
G_{au}^{u+}	2	-2	2	-2	0	1	-1	0	$i\sqrt{2}$	$-i\sqrt{2}$	0	1	-1	-2	2
G_{au}^{u-}	2	-2	2	-2	0	1	-1	0	$-i\sqrt{2}$	$i\sqrt{2}$	0	1	-1	-2	2
E_{1g}	2	2	-2	-2	2	2	2	0	0	0	-2	-2	-2	0	0
E_{2g}	2	2	-2	-2	2	-1	-1	0	0	0	-2	1	1	0	0
E_{3g}	2	2	-2	-2	2	-1	-1	0	0	0	-2	1	1	0	0
I_B	6	6	-6	-6	-2	0	0	0	0	0	2	0	0	0	0
G_{1aB}	4	-4	-4	4	0	2	-2	0	0	0	0	-2	2	0	0
G_{2aB}	4	-4	-4	4	0	-1	1	0	0	0	0	1	-1	0	0
G_{3aB}	4	-4	-4	4	0	-1	1	0	0	0	0	1	-1	0	0

O_h	E	A	AC	C^2, C	D	AD	BD	I
		B	BC	AC^2	ARD			
		AB	ABC	BC^2	C^2D	ABCD	ACD	
				ABC^2	AC^2D			
					HCD	BC^2D	ABC^2D	
					CD			

continues.....

$12c_4$	$8c_{12}$	$8c_{12}$	$8c_{12}$	$8c_{12}$	$24c_4$	$12c_8$	$12c_8$	192 elements
					ST, S ³ T	PST	QS ³ T	
					PQST, PQS ³ T	P ² QST	P ³ S ³ T	
					R ² ST, R ² S ³ T	PQRST	P ³ RS ³ T	
					PR ² ST, PR ² S ³ T	P ³ RST	P ³ QRS ³ T	
					QRST, QRS ³ T	QR ² ST	PQR ² S ³ T	
					P ² RST, P ² RS ³ T	P ³ QR ² ST	P ² QR ² ST	
PT, P ³ S ² T					P ² ST, P ² S ³ T	PS ³ T	QST	P ⁴ =Q ⁴ =R ³ =S ⁴ =T ⁴ =E
QT, P ² QS ² T					P ³ QST, P ³ QS ³ T	P ² QS ³ T	P ³ ST	P ² =Q ² ; S ² =T ²
PQT, P ³ QS ² T	PRT, P ³ QR ² S ² T	PRS ² T, P ³ QR ² T	R ² T, RS ² T	R ² S ² T, RT	P ² R ² ST, P ² R ² S ³ T	PQRS ³ T	P ³ RST	QP=P ³ Q; RP=QR; RQ=PQR
PS ² T, P ³ T	QRT, P ³ R ² S ² T	QRS ² T, P ³ R ² T	PR ² T, P ² QRS ² T	PR ² S ² T, P ² QRT	P ³ R ² ST, P ³ R ² S ³ T	P ³ RS ³ T	P ³ QRST	SP=P ² QS; SQ=P ³ S; SR=R ² S
QS ² T, P ² QT	PQRT, P ² QR ² S ² T	PQRS ² T, P ² QR ² T	QR ² T, P ³ QRS ² T	QR ² S ² T, P ³ QRT	P ² QRST, P ² QRS ³ T	QR ² S ³ T	PQR ² ST	TP=PT; TQ=QT; TR=RT
PQS ² T, P ³ QT	P ² RT, P ² R ² S ² T	P ² RS ² T, P ² R ² T	PQR ² T, P ³ RS ² T	PQR ² S ² T, P ³ RT	RST, RS ³ T	P ³ QR ² ST	P ² QR ² S ³ T	TS=S ³ T
1	1	1	1	1	1	1	1	} $\alpha=+1; \beta=+1$
1	1	1	1	1	-1	-1	-1	
2	-1	-1	-1	-1	0	0	0	
-1	0	0	0	0	-1	1	1	
-1	0	0	0	0	1	-1	-1	
-1	-1	-1	-1	-1	-1	-1	-1	
-1	-1	-1	-1	-1	1	1	1	
-2	1	1	1	1	0	0	0	
1	0	0	0	0	1	-1	-1	
1	0	0	0	0	-1	1	1	
0	-1	-1	1	1	0	0	0	
0	1	1	-1	-1	0	0	0	
0	1	1	-1	-1	0	$i\sqrt{2}$	$-i\sqrt{2}$	
0	1	1	-1	-1	0	$-i\sqrt{2}$	$i\sqrt{2}$	
0	-1	-1	1	1	0	$-i\sqrt{2}$	$i\sqrt{2}$	
0	-1	-1	1	1	0	$i\sqrt{2}$	$-i\sqrt{2}$	
0	0	0	0	0	0	0	0	
0	$-\sqrt{3}$	$\sqrt{3}$	$\sqrt{3}$	$-\sqrt{3}$	0	0	0	} $\beta=-1; \alpha=+1$
0	$\sqrt{3}$	$-\sqrt{3}$	$-\sqrt{3}$	$\sqrt{3}$	0	0	0	
0	0	0	0	0	0	0	0	} $\alpha=-1; \beta=-1$
0	$-\sqrt{3}$	$\sqrt{3}$	$-\sqrt{3}$	$\sqrt{3}$	0	0	0	
0	$\sqrt{3}$	$-\sqrt{3}$	$\sqrt{3}$	$-\sqrt{3}$	0	0	0	
AI	ACI		C ² I	CI	DI	ADI	BI	A ² -B ² -C ³ -D ² -I ² -E
BI	BCI		AC ² I		ABDI			BA=AB; CA=BC; CB=AC
ABI	ABCI		BC ² I		C ² DI	ABCDI	ACDI	DA=BD; DB=AD; DC=C ² D;
			ABC ² I		AC ² DI			IA=AI; IB=BI; IC=CI;
					BCDI	BC ² DI	ABC ² DI	ID=DI
					CDI			

$\mathcal{R}_4(O_h)$	$1e_1$	$1e_2$	$1e_2$	$1e_2$	$6e_4$	$8e_6$	$8e_3$	$24e_4$	$12e_8$	$12e_8$	$6e_4$	$8e_6$	$8e_6$	$2e_4$	$2e_4$	
	E	P ²	S ²	P ² S ²	PQ, P ³ Q	P ² R, P ² R ²	PQR ² , P ³ R	RS, RS ³	P ³ QR ² S	P ² QR ² S ³	PQS ² , P ³ QS ²	P ² RS ² , P ² R ² S ²	PQR ² S ² , P ³ RS ²	T	P ² T	
A_{1g}	1	1	1	1	1	1	1	1	1	1	1	1	1	1	1	
A_{2g}	1	1	1	1	1	1	1	-1	-1	-1	1	1	1	1	1	
E_g	2	2	2	2	2	-1	-1	0	0	0	2	-1	-1	2	2	
T_{1g}	3	3	3	3	-1	0	0	-1	1	1	-1	0	0	3	3	
T_{2g}	3	3	3	3	-1	0	0	1	-1	-1	-1	0	0	3	3	
A_{1u}	1	1	1	1	1	1	1	1	1	1	1	1	1	-1	-1	
A_{2u}	1	1	1	1	1	1	1	-1	-1	-1	1	1	1	-1	-1	
E_u	2	2	2	2	2	-1	-1	0	0	0	2	-1	-1	-2	-2	
T_{1u}	3	3	3	3	-1	0	0	-1	1	1	-1	0	0	-3	-3	
T_{2u}	3	3	3	3	-1	0	0	1	-1	-1	-1	0	0	-3	-3	
G_a	4	-4	4	-4	0	2	-2	0	0	0	0	2	-2	0	0	
K_a	K_a^+	4	-4	4	-4	0	-1	1	0	0	0	-1	1	0	0	
	K_a^-	4	-4	4	-4	0	-1	1	0	0	0	-1	1	0	0	
E_B	2	2	-2	-2	2	2	2	0	0	0	-2	-2	-2	0	0	
G_B	G_B^+	2	2	-2	-2	2	-1	-1	0	0	0	-2	1	1	0	0
	G_B^-	2	2	-2	-2	2	-1	-1	0	0	0	-2	1	1	0	0
I_B	6	6	-6	-6	-2	0	0	0	0	0	2	0	0	0	0	
G_{1aB}	G_{1aB}^+	2	-2	-2	2	0	1	-1	0	$-i\sqrt{2}$	$i\sqrt{2}$	0	-1	1	$2i$	$-2i$
	G_{1aB}^-	2	-2	-2	2	0	1	-1	0	$i\sqrt{2}$	$-i\sqrt{2}$	0	-1	1	$-2i$	$2i$
G_{2aB}	G_{2aB}^+	2	-2	-2	2	0	1	-1	0	$i\sqrt{2}$	$-i\sqrt{2}$	0	-1	1	$2i$	$-2i$
	G_{2aB}^-	2	-2	-2	2	0	1	-1	0	$-i\sqrt{2}$	$i\sqrt{2}$	0	-1	1	$-2i$	$2i$
K_{aB}	K_{aB}^+	4	-4	-4	4	0	-1	1	0	0	0	1	-1	$4i$	$-4i$	
	K_{aB}^-	4	-4	-4	4	0	-1	1	0	0	0	1	-1	$-4i$	$4i$	

O_h	E	A	AC	C ² , C	D	AD	BD	I
		B	BC	AC ²	ABD			
		AB	ABC	BC ²	C ² D	ABCD	ACD	
				ABC ²	AC ² D			
					BCD	BC ² D	ABC ² D	
					CD			

continues.....

$12e_2$	$8e_{12}$	$8e_{12}$	$8e_{12}$	$8e_{12}$	$24e_4$	$12e_8$	$12e_8$	192 elements	
PT					ST, P ² ST				
QT					PQST, P ³ QST				
PQT					R ² ST, P ² R ² ST				
PS ² T					PK ² ST, P ³ R ² ST				
QS ² T	PRT	PQR ² T	P ² R ² T	RT	QRST, P ² QRST				
PQS ² T	QRT	PR ² T	P ³ R ² T	P ² QRT	P ² RST, RST				
P ³ T	PQRT	QR ² T	P ² QR ² T	P ³ QRT	S ³ T, P ² S ³ T	PST, P ² QST	QST, P ³ ST	P ⁴ =Q ⁴ =R ⁴ =S ⁴ =T ⁴ =E	
P ² QT	P ² RT	R ² T	P ³ QR ² T	P ³ RT	PQS ³ T, P ³ QS ³ T	PQRST, P ³ RST	PRST, P ³ QRST	P ² =Q ² =T ²	
P ³ QT	P ² R ² S ² T	RS ² T	PRS ² T	PQR ² S ² T	R ² S ³ T, P ² R ² S ³ T	QR ² ST, P ³ QR ² ST	PQR ² ST, P ² QR ² ST	QP=P ³ Q; RP=QR; RQ=PQR	
P ³ S ² T	P ³ R ² S ² T	P ² QRS ² T	QRS ² T	PR ² S ² T	PR ² S ³ T, P ³ R ² S ³ T	PS ³ T, P ² QS ³ T	QS ³ T, P ³ S ³ T	SP=P ² QS; CQ=P ³ S; SR=R ² S	
P ² QS ² T	P ² QR ² S ² T	P ³ QRS ² T	PQRS ² T	QR ² S ² T	QRS ³ T, P ² QRS ³ T	PQRS ³ T, P ³ RS ³ T	PRS ³ T, P ³ QRS ³ T	TP=PT; TQ=QT; TR=RT	
P ³ QS ² T	P ³ QR ² S ² T	P ³ RS ² T	P ² RS ² T	R ² S ² T	P ² RS ³ T, PS ³ T	QR ² S ³ T, P ³ QR ² S ³ T	PQR ² S ³ T, P ² QR ² S ³ T	TS=S ³ T	
1	1	1	1	1	1	1	1	} $\alpha=+1; \beta=+1$	
1	1	1	1	1	-1	-1	-1		
2	-1	-1	-1	-1	0	0	0		
-1	0	0	0	0	-1	1	1		
-1	0	0	0	0	1	-1	-1		
-1	-1	-1	-1	-1	-1	-1	-1		
-1	-1	-1	-1	-1	1	1	1		
-2	1	1	1	1	0	0	0		
1	0	0	0	0	1	-1	-1		
1	0	0	0	0	-1	1	1		
0	0	0	0	0	0	0	0		
0	-i/3	i/3	-i/3	i/3	0	0	0		} $\alpha=-1; \beta=+1$
0	i/3	-i/3	i/3	-i/3	0	0	0		
0	0	0	0	0	0	0	0		
0	-i/3	i/3	i/3	-i/3	0	0	0		} $\alpha=+1; \beta=-1$
0	i/3	-i/3	-i/3	i/3	0	0	0		
0	0	0	0	0	0	0	0		
0	i	-i	i	-i	0	√2	-√2	} $\alpha=-1; \beta=-1$	
0	-i	i	-i	i	0	√2	-√2		
0	i	-i	i	-i	0	-√2	√2		
0	-i	i	-i	i	0	-√2	√2		
0	-i	i	-i	i	0	0	0		
0	i	-i	i	-i	0	0	0		
AI	ACI		C ² I	CI	DI	ADI	BDI	A ² =B ² =C ² =D ² =I ² =E	
BI	BCI		AC ² I		ABDI	ARCDI	ACDI	BA=AB; CA=BC; CB=ABC	
ABI	ABCI		ABC ² I		C ² DI	BC ² DI	ABC ² DI	DA=BD; DB=AD; EC=C ² D;	
					AC ² DI			IA=AI; IB=BI; IC=CI;	
					BCDI			ID=DI.	
					CDI				

$1e_1$ $1e_2$	$30e_4$	$20e_6$	$20e_3$	$12e_5$	$12e_5$	$12e_{10}$	$12e_{10}$	120 elements
R (1)	<p>P, P³ Q, P²Q PQ, P³Q PV, P³V PV², P³V² PV³, P³V³ PV⁴, P³V⁴ PRV², P³RV² PR²V², P³R²V² PQR²V, PR²V⁴ QV, R²V³ PQR²V³, P³QR²V³ PQR²V⁴, P³QR²V⁴ RV, P²RV R²V⁴, P²R²V⁴ QRV³, P²QRV³ P²R, P²R² P²QRV, P³QV²</p>	<p>PR, P³QR² QR, P³R² PQR, P²QR² PQR²V, PR²V⁴ QV, R²V³ PQR²V³, P³QR²V³ QR²V², P²QV⁴ RV², P³QRV³ P²R, P²R² P²QRV, P³QV²</p>	<p>R, R² PR², P²QR PQR², P³R QR², P³QR QV⁴, P²QR²V² PQV², P²QRV⁴ PQRV³, P²RV² PRV⁴, P³QV³ P²QV, P²R²V³ P²R²V⁴, P³QR²V² P²QRV, P³QV²</p>	<p>V, V⁴ QV², P²RV⁴ RV³, P²QR²V⁴ PQRV, P²QV³ R²V², QR²V³ P²R²V³, P³QRV² P²R²V⁴, P³QV⁴</p>	<p>V², V³ PQV, P³QR²V² QRV², PQR²V⁴ PRV³, P²RV³ P³RV, P²QRV⁴ P³R²V³, P³QV⁴</p>	<p>QV³, P³QRV R²V, PQRV² RV⁴, P²QV² QR²V⁴, P²RV³ P²V, P²V⁴ P²R²V², P²QR²V³ P³R²V, P³RV³</p>	<p>PRV, QRV⁴ PR²V³, PQRV⁴ PQR²V², P³QV P²V², P²V³ P²QRV², P³QR²V⁴ P³R²V, P³RV³</p>	<p>P⁴=Q⁴=R³=V⁵=E Q²=P² QP=P³Q; RP=QR RQ=PQR; VP=PV⁴ VQ=QR²V²; VR=P²R²V⁴</p>
A	1	1	1	1	1	1	1	} $\alpha=+1$
T ₁	3	0	0	ϕ^{-1}	ϕ^{-1}	ϕ	ϕ^{-1}	
T ₂	3	0	0	ϕ^{-1}	ϕ	ϕ^{-1}	ϕ	} $\alpha=-1$
G	4	1	1	-1	-1	-1	-1	
H	5	1	-1	0	0	0	0	
E ₁	2	-2	1	-1	-1	ϕ^{-1}	ϕ^{-1}	
E ₂	2	-2	1	-1	-1	ϕ^{-1}	ϕ^{-1}	
C ₂	4	-4	1	-1	1	1	-1	
I ₂	6	-6	0	0	-1	-1	1	
I	<p>A B AB AF AF² AF³ AF⁴ ACF² AC²F² ABCF⁴ ABC²F³ CF C²F⁴ BCF³ BC²F</p>	<p>AC BC ABC ABC²F, AC²F⁴ BF, C²F³ ABF⁵ BC²F² CF²</p>	<p>C, C² AC² ABC² EC² BF⁴ ASF², BCF ABC²F³ ACF⁴</p>	<p>F, F⁴ EF² CF³ ABCF C²F², BC²F³</p>	<p>F², F³ ABF BCF², ABC²F⁴ ACF³, AC²F</p>	<p>BF³ C²F, ABCF² CF⁴ BC²F⁴</p>	<p>ACF, BCF⁴ AC²F³, ABV⁴ ABC²F²</p>	<p>A²=B²=C³=F⁵=E BA=AB; CA=BC CB=ABC; FA=AF⁴ FB=BC²F²; FC=C²F⁴</p>

$\phi = 1(\sqrt{5}+1); \phi^{-1} = 1(\sqrt{5}-1)$

A_E	1	1	1	1	1	1	1	1	1	1	1	1	1	1	1	1	1	1	
T_{1g}	3	3	-1	0	0	ϕ	ϕ^{-1}	ϕ	ϕ^{-1}	3	3	-1	0	0	ϕ	ϕ^{-1}	ϕ	ϕ^{-1}	
T_{2g}	3	3	-1	0	0	ϕ^{-1}	ϕ	ϕ^{-1}	ϕ	3	3	-1	0	0	ϕ^{-1}	ϕ	ϕ^{-1}	ϕ	
G_g	4	4	0	1	1	-1	-1	-1	-1	4	4	0	1	1	-1	-1	-1	-1	
H_g	5	5	1	-1	-1	0	0	0	0	5	5	1	-1	-1	0	0	0	0	
A_u	1	1	1	1	1	1	1	1	1	-1	-1	-1	-1	-1	-1	-1	-1	-1	$\omega=1$
T_{1u}	3	3	-1	0	0	ϕ	ϕ^{-1}	ϕ	ϕ^{-1}	-3	-3	1	0	0	$-\phi$	$-\phi^{-1}$	$-\phi$	$-\phi^{-1}$	
T_{2u}	3	3	-1	0	0	ϕ^{-1}	ϕ	ϕ^{-1}	ϕ	-3	-3	1	0	0	$-\phi^{-1}$	$-\phi$	$-\phi^{-1}$	$-\phi$	
G_u	4	4	0	1	1	-1	-1	-1	-1	-4	-4	0	-1	-1	1	1	1	1	
H_u	5	5	1	-1	-1	0	0	0	0	-5	-5	-1	1	1	0	0	0	0	
C_{1a}	C_{1a}^+	2	-2	0	1	-1	-1	ϕ	ϕ^{-1}	2i	-2i	0	i	-i	-i ϕ	i ϕ	-i ϕ^{-1}	i ϕ^{-1}	
	C_{1a}^-	2	-2	0	1	-1	-1	$-\phi$	$-\phi^{-1}$	-2i	2i	0	-i	i	i ϕ	-i ϕ	i ϕ^{-1}	-i ϕ^{-1}	
C_{2a}	C_{2a}^+	2	-2	0	1	-1	-1	ϕ^{-1}	ϕ	2i	-2i	0	i	-i	i ϕ^{-1}	-i ϕ^{-1}	i ϕ	-i ϕ	
	C_{2a}^-	2	-2	0	1	-1	-1	ϕ^{-1}	ϕ	-2i	2i	0	-i	i	-i ϕ^{-1}	i ϕ^{-1}	-i ϕ	i ϕ	
X_a	X_a^+	4	-4	0	-1	1	-1	-1	1	4i	-4i	0	-i	i	-i	-i	i	i	$\omega=-1$
	X_a^-	4	-4	0	-1	1	-1	-1	1	-4i	4i	0	i	-i	i	i	-i	-i	
O_a	O_a^+	6	-6	0	0	0	1	1	-1	6i	-6i	0	0	0	i	i	-i	-i	
	O_a^-	6	-6	0	0	0	1	1	-1	-6i	6i	0	0	0	-i	-i	i	i	
I_h	E	A	AC	C, C^2	F, F^4	F^2, F^3	BP^3	ACP, BCP^4	I	AI	ACI	ABC^2I	FI	CF^4I	F^2I	ABC^2F^2I	$A^2-B^2-C^3-F^5-I^2-E$		
		B	BC	AC^2	BF^2	ABF	$C^2F, ABCF^2$	AC^2F^3, ABF^4		BI	BCI	AC^2I	F^4I	BC^2F^4I	F^3I	BCF^4I	$BA-AB; CA-BC$		
		AB	ABC	ABC^2	CF^3	BCF^2, ABC^2F^4	CF^4	ABC^2F^2		ABI	ABCI	EC^2I	BF^2I	BF^3I	ABFI	ACFI	$CB-AC; FA-AP^4$		
		AF	ABC^2F, AC^2F^4	BC^2	ABCF	ACF^3, AC^2F	BC^2F^4		AFI	ABC^2FI	ACF^4I	CF^3I	$ABCF^2I$	BCF^2I	ABF^4I	$FB-BC^2F^2; FC-C^2F^4$			
		AF^2	BF, C^2F^3	BF^4	C^2F^2, BC^2F^3				AF^2I	EFI	BF^4I	ABCFI	C^2FI	AEC^2F^4I	AC^2F^3I	$IA-AI; IB-BI$			
		AF^3	ABF^3	ABF^2, BCF					AF^3I	ABF^3I	ABC^3I	C^2F^2I		ACF^3I	$IC-CI; IF-FI$				
		AF^4	BC^2F^2	$ABCF^3$					AF^4I	BC^2F^2I	C^2I	BC^2F^3I		AC^2FI					
		ACP^2	CF^2	ACP^4					ACP^2I	CF^2I	ABF^2I								
		AC^2F^2							AC^2F^2I	AC^2F^4I	CI								
		$ABCF^4$							$ABCF^4I$	C^2F^3I	BCFI								
		ABC^2F^3							ABC^2F^3I										
		CF							CFI										
		C^2F^4							C^2F^4I										
		BCF^3							BCF^3I										
		BC^2F							BC^2FI										

$\phi = \frac{1}{2}(\sqrt{5} + 1); \quad \phi^{-1} = \frac{1}{2}(\sqrt{5} - 1)$

$R_1(K_h)$	E	∞C_∞^ϕ	R	S_2	σ_h	∞ elements
D_{jg}	$2j+1$	$1 + \sum_{\ell=1}^{\ell=j} 2\cos\ell\phi$	$2j+1$	$2j+1$	$(-1)^j$	} $\alpha=+1$
D_{ju}	$2j+1$	$1 + \sum_{\ell=1}^{\ell=j} 2\cos\ell\phi$	$2j+1$	$-2j-1$	$(-1)^{j+1}$	
$D_{(j+\frac{1}{2})g}$	$2j+2$	$\sum_{\ell=0}^{\ell=j+1} 2\cos(\ell+\frac{1}{2})\phi$	$-2j-2$	$2j+2$	0	} $\alpha=-1$
$D_{(j+\frac{1}{2})u}$	$2j+2$	$\sum_{\ell=0}^{\ell=j+1} 2\cos(\ell+\frac{1}{2})\phi$	$-2j-2$	$-2j-2$	0	
K_h	E	∞C_∞^ϕ		S_2	σ_h	

$\mathcal{R}_2(K_h)$	E	∞C_∞^ϕ	R	S_2	$\infty C_\infty^\phi S_2$	∞ elements
D_{jg}	$2j+1$	$1 + \sum_{\ell=1}^{\ell=j} 2\cos\ell\phi$	$2j+1$	$2j+1$	$1 + \sum_{\ell=1}^{\ell=j} 2\cos\ell\phi$	} $\alpha=+1$
D_{ju}	$2j+1$	$1 + \sum_{\ell=1}^{\ell=j} 2\cos\ell\phi$	$2j+1$	$-2j-1$	$-1 - \sum_{\ell=1}^{\ell=j} 2\cos\ell\phi$	
$D_{(j+\frac{1}{2})\alpha}$	$2j+2$	$\sum_{\ell=0}^{\ell=j+1} 2\cos(\ell+\frac{1}{2})\phi$	$-2j-2$	$2i(j+1)$	$\sum_{\ell=0}^{j+1} 2i\cos(\ell+\frac{1}{2})\phi$	} $\alpha=-1$
	$2j+2$	$\sum_{\ell=0}^{\ell=j+1} 2\cos(\ell+\frac{1}{2})\phi$	$-2j-2$	$-2i(j+1)$	$-\sum_{\ell=0}^{j+1} 2i\cos(\ell+\frac{1}{2})\phi$	
K_h	E	∞C_∞^ϕ		S_2	$\infty C_\infty^\phi S_2$	

CHAPTER 4

ASCENT AND DESCENT IN SYMMETRY AND SYMMETRIZED POWERS
FOR PROJECTIVE REPRESENTATIONS

4.1 ASCENT AND DESCENT IN SYMMETRY

The process of ascent and descent in symmetry (also known as induction and subduction) relates the vector representations of the point group, G , to those of a subgroup of G , due to the following reciprocity theorem of Frobenius (4.2).

Let D be a representation of a finite group G with character $\chi^D(g)$. Let H be a subgroup of G . Then the number of times that D will appear in the ascent of D^j to G into irreducible representations of G , is equal to the number of times the representation D^j appears in the descent of D to H .

G can be factorized into left cosets with respect to H :

$$G = \sum_{\alpha} \rho_{\alpha} H$$

where ρ_{α} are any left coset representatives. The number of times, n , that D appears in the ascent of D^j to G is equal to the intertwining number

$$n = \frac{1}{|G|} \sum_g \chi(g) \chi^D(g^{-1})$$

Then the elements of G may be expressed in the following way

$$n = \frac{1}{|G|} \sum_h \sum_{\alpha} \chi^j(h) \chi^D(\rho_{\alpha} h^{-1} \rho_{\alpha}^{-1})$$

But h^{-1} and $\rho_{\alpha} h^{-1} \rho_{\alpha}^{-1}$ are in the same conjugacy class of G and so have the same character $\chi^D(h^{-1})$ for all values of α from 1 to $|G|/|H|$.

Therefore

$$n = \frac{1}{|H|} \sum_h \chi^j(h) \chi^D(h^{-1})$$

with the condition that D is irreducible in G and D^j is irreducible in H .

This is a well-known process for relating representations of a supergroup to a subgroup. Relations between the projective representations of

G and H are in general, however, severely restricted, not only by differences in the multipliers but also by the choice of representation group. Indeed for specific physical problems it may be advantageous to choose a particular representation group and hence a particular set of projective representations, to facilitate the process of descent in symmetry.

To quote specific examples, the representation groups of O_h and D_{4h} are respectively of orders 192 and 128 and hence the projective representations of O_h cannot be subduced onto those of D_{4h} even though D_{4h} is a maximal subgroup of O_h . This is clearly because the multiplier of D_{4h} is of greater order than that of O_h .

Further, of the two representation groups of D_2 , only $R_1(D_2)$ is a subgroup of $R(T)$ and hence there is clearly some advantage to be gained in dealing with the projective representations of D_2 derived from $R_1(D_2)$ rather than those derived from $R_2(D_2)$ when descent for the tetrahedral group is of interest.

Descents in symmetry are sometimes possible when the order of the multiplier decreases from G_1 to G_2 . For example, the multiplier of O_h is of order four while that of O , T_d , T_h and D_{3d} is of order two. However, only from $R_1(O_h)$ and $R_2(O_h)$ is a descent possible to a representation group of each of these four groups.

The only descents to maximal subgroups presented are those to maximal subgroups which are themselves representation groups of a point group. This includes cases where the multiplier is necessarily trivial so that formally the point group is its own representation group. The correlations obey all of Frobenius's rules, therefore only descents to maximal subgroups have been presented in the following tables. The complete set of descents in symmetry from a supergroup to all possible subgroups are presented, where the dotted lines in the diagrams indicate that the descent in symmetry

continues in the above way until the trivial group C_1 is obtained.

The consideration of different representation groups for a group G leads to more complete and detailed results than those obtainable by Harter (43).

4.I.I Correlation Tables

4.I.I Correlation Tables

$R_1(C_{4nh})$	C_{4n}	$R_1(C_{(4n-2)h})$	C_{4n-2}	$C_{(2n-1)h}$	$R_1(C_{2h})$
A_g	A	A_g	A	A'	A_g
A_u	A	A_u	A	A'	A_u
B_g	B	B_g	B	A''	B_g
B_u	B	B_u	B	A''	B_u
E_{lg}	E_l	E_{lg}	E_l	$\begin{cases} l \text{ odd: } E''_{n-\frac{1}{2}l-\frac{1}{2}} \\ l \text{ even: } E'_{\frac{1}{2}l} \end{cases}$	$2B_g$
E_{lu}	E_l	E_{lu}	E_l		$2A_g$
$E_{\frac{n}{2}\alpha}$	$E_{\frac{n}{2}\alpha}$	E_{lu}	E_l	$\begin{cases} l \text{ odd: } E''_{n-\frac{1}{2}l-\frac{1}{2}} \\ l \text{ even: } E'_{\frac{1}{2}l} \end{cases}$	$2B_u$
$E_{n\alpha}$	A+B	$E_{n\alpha}$	A+B		$2A_u$
$G_{l\alpha}$	$E_l + E_{2n-l}$	$G_{l\alpha}$	$E_l + E_{2n-l-1}$	$A' + A''$	$E_{l\alpha}$
				$E'_l + E''_l$	$2E_{l\alpha}$

$R_2(C_{4nh})$	C_{4n}	$R_2(C_{(4n-2)h})$	C_{4n-2}	$C_{(2n-1)h}$	$R_2(C_{2h})$
A_g	A	A_g	A	A'	A_g
A_u	A	A_u	A	A'	A_u
B_g	A	B_g	A	A'	B_g
B_u	A	B_u	A	A'	B_u
$l \neq n; E_{lg}$	$E_{(2n- 2n-2l) \bmod 2n}$	E_{lg}	$E_{(2n-1- 2n-2l-1) \bmod (2n-1)}$	$E'_{n-\frac{1}{2}- n-\frac{1}{2}-l \bmod n }$	$\begin{cases} l \text{ odd: } 2B_g \\ l \text{ even: } 2A_g \end{cases}$
$l \neq n; E_{lu}$	$E_{(2n- 2n-2l) \bmod 2n}$	E_{lu}	$E_{(2n-1- 2n-2l-1) \bmod (2n-1)}$	$E'_{n-\frac{1}{2}- n-\frac{1}{2}-l \bmod n }$	$\begin{cases} l \text{ odd: } 2B_u \\ l \text{ even: } 2A_u \end{cases}$
E_{ng}	2B				
E_{nu}	2B				
$G_{l\alpha}$	$2E_{2l-1}$	E_α	2B	$2A''$	E_α
		$G_{l\alpha}$	$2E_{2l-1}$	$2E''_l$	$2E_\alpha$

Table I. Correlation of the irreducible representations of the C_{2nh} groups with those of their maximal subgroups.

$\mathcal{R}_1(D_{2n})$	C_{2n}	n odd ($\neq 1$) $\mathcal{R}_1(D_2)$	n even $\mathcal{R}_1(D_n)$
A_1	A	A_1	A_1
A_2	A	A_2	A_2
B_1	A	B_1	A_1
B_2	A	B_2	A_2
$l \neq n; E_l$	$E_{n- n-2l \bmod n }$	$\begin{cases} l \text{ odd: } B_1+B_2 \\ l \text{ even: } A_1+A_2 \end{cases}$	$E_{n- n-l \bmod \frac{1}{2}n}$
E_n	$2B$	$\begin{cases} l \text{ odd: } B_1+B_2 \\ l \text{ even: } A_1+A_2 \end{cases}$	B_1+B_2
$E_{l\alpha}$	$E_{n- n-(2l-1) \bmod 2n \bmod n}$	$E_{l\alpha}$	$E_{\{n+\frac{1}{2}- n+\frac{1}{2}-l \bmod 2n\}\alpha}$

$\mathcal{R}_2(D_{2n})$	C_{2n}	n odd D_n	n even $\mathcal{R}_2(D_n)$	n odd ($\neq 1$) $\mathcal{R}_2(D_2)$
A_1	A	A_1	A_1	A_1
A_2	A	A_2	A_2	A_2
B_1	A	A_1	A_1	B_1
B_2	A	A_2	A_2	B_2
$l \neq n; E_l$	$E_{n- n-2l \bmod n }$	$E_{\frac{1}{2}n- \frac{1}{2}n-2l \bmod n }$	$E_{n- n-l \bmod \frac{1}{2}n}$	$\begin{cases} l \text{ odd: } B_1+B_2 \\ l \text{ even: } A_1+A_2 \end{cases}$
E_n	$2B$	$E_{\frac{1}{2}n- \frac{1}{2}n-2l \bmod n }$	B_1+B_2	$\begin{cases} l \text{ odd: } B_1+B_2 \\ l \text{ even: } A_1+A_2 \end{cases}$
$l \neq \frac{1}{2}n + \frac{1}{2}; E_{l\alpha}$	$E_{n- n-(2l-1) \bmod 2n \bmod n}$	$E_{n- n+1-2l \bmod n }$	$E_{\{n+\frac{1}{2}- n+\frac{1}{2}-l \bmod 2n\}\alpha}$	$E_{l\alpha}$
$E_{\{\frac{1}{2}n+\frac{1}{2}\}\alpha}$	$E_{n- n-(2l-1) \bmod 2n \bmod n}$	A_1+A_2	$E_{\{n+\frac{1}{2}- n+\frac{1}{2}-l \bmod 2n\}\alpha}$	$E_{l\alpha}$

$\mathcal{R}_3(D_{4n-2})$	C_{4n-2}	D_{2n-1}	$n \neq 1$ $\mathcal{R}_2(D_2)$
A_1	A	A_1	A_1
A_2	A	A_2	B_1
B_1	B	A_2	A_2
B_2	B	A_1	B_2
E_l	E_l	$E_{n-\frac{1}{2}- n-l-\frac{1}{2} }$	$\begin{cases} l \text{ odd: } A_2+B_2 \\ l \text{ even: } A_1+B_1 \end{cases}$
E_α	$A+B$	A_1+A_2	$E_{l\alpha}$
$G_{l\alpha}$	$E_{2l}+E_{2n-2l-1}$	$2E_{n-\frac{1}{2}- n-\frac{1}{2}-2l \bmod 2n }$	$2E_{l\alpha}$

$\mathcal{R}_3(D_{4n})$	C_{4n}	$\mathcal{R}_1(D_{2n})$	$\mathcal{R}_2(D_{2n})$
A_1	A	A_1	A_1
A_2	A	A_1	A_2
B_1	A	A_2	A_1
B_2	A	A_2	A_2
$l \neq n; E_l$	$E_{2n- 2n-2l \bmod 2n}$	$E_{n- n-l \bmod n}$	$E_{n- n-l \bmod n}$
E_n	$2B$	B_1+B_2	B_1+B_2
$G_{l\alpha}$	$E_{2n- 2n-2l+1 }$	$2E_{\{n+\frac{1}{2}- n-(l-\frac{1}{2}) \bmod 2n\}\alpha}$	$2E_{\{n+\frac{1}{2}- n-(l-\frac{1}{2}) \bmod 2n\}\alpha}$

Table 2. Correlation of the irreducible representations of the representation groups of the dihedral groups D_{2n} with those of their maximal subgroups.

$R_1(D_{(4n+2)h})$	$R(D_{2n})$	$R_2(D_{(4n+2)h})$	$R(D_{2n})$
A_{1g}	A_{1g}	A_{1g}	A_{1g}
A_{1u}	A_{1u}	A_{1u}	A_{1u}
A_{2g}	A_{2g}	A_{2g}	A_{2g}
A_{2u}	A_{2u}	A_{2u}	A_{2u}
B_{1g}	B_{1g}	B_{1g}	B_{1g}
B_{1u}	B_{1u}	B_{1u}	B_{1u}
B_{2g}	B_{2g}	B_{2g}	B_{2g}
B_{2u}	B_{2u}	B_{2u}	B_{2u}
E_{1g}	$\begin{cases} l \text{ odd: } B_{1g} + B_{2g} \\ l \text{ even: } A_{1g} + A_{2g} \end{cases}$	E_{1g}	$\begin{cases} l \text{ odd: } B_{1u} + B_{2u} \\ l \text{ even: } A_{1g} + A_{2g} \end{cases}$
E_{1u}	$\begin{cases} l \text{ odd: } B_{1u} + B_{2u} \\ l \text{ even: } A_{1u} + A_{2u} \end{cases}$	E_{1u}	$\begin{cases} l \text{ odd: } B_{1g} + B_{2g} \\ l \text{ even: } A_{1u} + A_{2u} \end{cases}$
E_{1x}	$\begin{cases} l \text{ odd: } E_{1x} \\ l \text{ even: } E_{2x} \end{cases}$	E_{1x}	E_{1x}
E_{2x}	E_{2x}	E_{2x}	E_{2x}
$E_{1\beta}$	$E_{1\beta}$	G_{2x}	$E_{1x} + E_{2x}$
$E_{2\beta}$	$E_{2\beta}$	$E_{1\beta}$	$E_{1\beta}$
$G_{2\beta}$	$\begin{cases} l \text{ odd: } 2E_{2\beta} \\ l \text{ even: } 2E_{1\beta} \end{cases}$	$E_{2\beta}$	$E_{2\beta}$
E_{1x}	E_{1x}	$G_{2\beta}$	$E_{1\beta} + E_{2\beta}$
E_{2x}	E_{2x}	E_{1x}	E_{1x}
G_{2x}	$E_{1x} + E_{2x}$	E_{2x}	E_{2x}
$G_{1\alpha\beta}$	$G_{1\alpha\beta}$	G_{2x}	$E_{1x} + E_{2x}$
G_{2x}	G_{2x}	$G_{2\alpha\beta}$	$G_{1\alpha\beta}$
$G_{2\alpha}$	$G_{2\alpha}$	E_{2x}	E_{2x}
$G_{2\alpha}$	$G_{2\alpha}$	$G_{2\alpha}$	$2E_{2\alpha}$
G_{β}	G_{β}	E_{β}	E_{β}
$G_{2\beta}$	$G_{2\beta}$	$G_{2\beta}$	$2E_{2\beta}$
$E_{1\alpha\beta}$	$E_{1\alpha\beta}$	$E_{2\alpha\beta}$	$\begin{cases} l \text{ odd: } E_{1\alpha\beta} \\ l \text{ even: } E_{2\alpha\beta} \end{cases}$
$E_{2\alpha\beta}$	$E_{2\alpha\beta}$		
$G_{1\alpha\beta}$	$E_{1\alpha\beta} + E_{2\alpha\beta}$		

Table 3. Correlation of the irreducible representations of the representation groups of the D_{2nh} groups with those of their maximal subgroups. The D_{4nh} groups have no representation groups as maximal subgroups.

$\mathcal{R}(T)$	$\mathcal{R}_1(D_2)$	C_3
A	A_1	A
E	$2A_1$	E
T	$A_2+B_1+B_2$	A+E
$E_{\frac{1}{2}}$	$E_{1\kappa}$	E
$G_{\frac{3}{2}}$	$2E_{1\kappa}$	$2A+E$

$\mathcal{R}_1(T_h)$	$\mathcal{R}(T)$	S_6	$\mathcal{R}_2(T_h)$	$\mathcal{R}(T)$	S_6
A_g	A	A_g	A_g	A	A_g
A_u	A	A_u	A_u	A	A_g
E_g	E	E_g	E_g	E	E_g
E_u	E	E_u	E_u	E	E_g
T_g	T	A_g+E_g	T_g	T	A_g+E_g
T_u	T	A_u+E_u	T_u	T	A_g+E_g
$E_{\frac{1}{2}g}$	$E_{\frac{1}{2}}$	E_g	G_{α}	$2E_{\frac{1}{2}}$	$2E_u$
$E_{\frac{1}{2}u}$	$E_{\frac{1}{2}}$	E_u	G'_{α}	$G_{\frac{3}{2}}$	$2A_u+E_u$
$G_{\frac{3}{2}g}$	$G_{\frac{3}{2}}$	$2A_g+E_g$	G''_{α}	$G_{\frac{3}{2}}$	$2A_u+E_u$
$G_{\frac{3}{2}u}$	$G_{\frac{3}{2}}$	$2A_u+E_u$			

Table 4. Correlation of the irreducible representations of the representation groups of the tetrahedral groups with their maximal subgroups. The two representation groups of the regular tetrahedral group (T_d) are isomorphic with those of the octahedral rotation group (O), q.v. The tables for $\mathcal{R}_1(O)$ and $\mathcal{R}_2(O)$ should therefore be used, with the corresponding changes in the subgroups, viz. $\mathcal{R}(D_4) \rightarrow \mathcal{R}(D_{2d})$ and $D_3 \rightarrow C_{3v}$.

A_1	A	A_1	A_1	A_1	A	A_1	A_1
A_2	A	B_2	A_2	A_2	A	B_2	A_2
E	E	A_1+B_2	E	E	E	A_1+B_2	E
T_1	T	A_2+E	T_1	T	A_2+E_1	A_2+E	A_2+E
T_2	T	B_1+E	T_2	T	B_1+E_1	A_1+E	A_1+E
$E_{\frac{1}{2}}$	$E_{\frac{1}{2}}$	$E_{1\alpha}$	$G_{\frac{1}{2}}$	$2E_{\frac{1}{2}}$	$E_{1\alpha}$	2E	2E
$E_{\frac{3}{2}}$	$E_{\frac{1}{2}}$	$E_{2\alpha}$	$G_{\frac{3}{2}}$	$G_{\frac{3}{2}}$	$E_{2\alpha}$	A_1+A_2+E	A_1+A_2+E
$G_{\frac{3}{2}}$	$G_{\frac{3}{2}}$	$E_{1\alpha}+E_{2\alpha}$					

$\mathcal{R}_1(O_h)$	$\mathcal{R}_1(O)$	$\mathcal{R}_1(T_h)$	$\mathcal{R}_3(D_{3d})$	$\mathcal{R}_2(O_h)$	$\mathcal{R}_2(O)$	$\mathcal{R}_1(T_h)$	$\mathcal{R}_2(D_{3d})$	$\mathcal{R}_3(O_h)$	$\mathcal{R}_1(T_h)$	$\mathcal{R}_2(D_{3d})$	$\mathcal{R}_1(O_h)$	$\mathcal{R}_1(T_h)$	$\mathcal{R}_2(T_h)$
A_{1g}	A_1	A_g	A_1	A_{1g}	A_1	A_g	A_1	A_{1g}	A_g	A_1	A_{1g}	A_g	A_g
A_{1u}	A_2	A_u	B_1	A_{1u}	A_1	A_g	B_1	A_{1u}	A_g	B_1	A_{1u}	A_g	A_u
A_{2g}	A_2	A_g	A_2	A_{2g}	A_2	A_g	A_2	A_{2g}	A_g	A_2	A_{2g}	E_g	A_g
A_{2u}	A_2	A_u	B_2	A_{2u}	A_2	A_g	B_2	A_{2u}	A_g	B_2	A_{2u}	T_g	A_u
E_g	E	E_g	E_2	E_g	E	E_g	E_2	E_g	E_g	E_2	E_g	T_g	E_g
E_u	E	E_u	E_1	E_u	E	E_g	E_1	E_u	E_g	E_1	E_u	A_g	E_u
T_{1g}	T_1	T_g	A_2+E_2	T_{1g}	T_1	T_g	A_2+E_2	T_{1g}	T_g	A_2+E_2	T_{1g}	A_g	T_g
T_{1u}	T_1	T_u	B_2+E_1	T_{1u}	T_1	T_g	B_2+E_1	T_{1u}	T_g	B_1+E_1	T_{1u}	E_g	T_u
T_{2g}	T_2	T_g	A_1+E_2	T_{2g}	T_2	T_g	A_1+E_2	T_{2g}	T_g	A_1+E_2	T_{2g}	T_g	T_g
T_{2u}	T_2	T_u	B_1+E_1	T_{2u}	T_2	T_g	B_1+E_1	T_{2u}	T_g	B_2+E_1	T_{2u}	T_g	T_u
G_{α}	$E_{\frac{1}{2}}+E_{\frac{3}{2}}$	$2E_{\frac{1}{2}g}$	$G_{1\alpha}$	$G'_{\alpha g}$	$G_{\frac{3}{2}}$	$G_{\frac{3}{2}g}$	$A_1+A_2+E_2$	$G'_{\alpha g}$	$G_{\frac{3}{2}g}$	$B_1+B_2+E_1$	G_{α}	$2E_{\frac{1}{2}g}$	G_{α}
K_{α}	$2G_{\frac{3}{2}}$	$2G_{\frac{3}{2}g}$	$2E_{\alpha}+G_{1\alpha}$	$G'_{\alpha u}$	$G_{\frac{3}{2}}$	$G_{\frac{3}{2}g}$	$B_1+B_2+E_1$	$G'_{\alpha u}$	$G_{\frac{3}{2}g}$	$A_1+A_2+E_2$	K_{α}	$2A_u$	$G'_{\alpha}+G_{\alpha}$
E_{β}	A_1+A_2	$2A_u$	E_{α}	$G''_{\alpha g}$	$G_{\frac{1}{2}}$	$2E_{\frac{1}{2}g}$	$2E_2$	$G''_{\alpha g}$	$2E_{\frac{1}{2}g}$	$2E_1$	E_{β}	$2A_u$	A_g+A_u
G_{β}	2E	$2E_u$	$G_{1\alpha}$	$G''_{\alpha u}$	$G_{\frac{1}{2}}$	$2E_{\frac{1}{2}g}$	$2E_1$	$G''_{\alpha u}$	$2E_{\frac{1}{2}g}$	$2E_2$	G_{β}	$2E_u$	E_g+E_u
I_{β}	T_1+T_2	$2T_u$	$E_{\alpha}+G_{1\alpha}$	$E_{1\beta}$	A_1+A_2	$2A_u$	$E_{2\alpha}$	$E_{1\beta}$	$2A_u$	$E_{2\alpha}$	I_{β}	$2T_u$	T_g+T_u
$E'_{\alpha\beta g}$	$E_{\frac{1}{2}}$	$E_{\frac{1}{2}u}$	E_2	$E_{2\beta}$	E	E_u	$E_{3\alpha}$	$E_{2\beta}$	E_u	$E_{3\alpha}$	$G_{1\alpha\beta}$	$2E_{\frac{1}{2}u}$	G_{α}
$E''_{\alpha\beta u}$	$E_{\frac{3}{2}}$	$E_{\frac{1}{2}u}$	E_1	$E_{3\beta}$	E	E_u	$E_{1\alpha}$	$E_{3\beta}$	E_u	$E_{1\alpha}$	$G_{2\alpha\beta}$	$G_{\frac{3}{2}u}$	G_{α}
$E'''_{\alpha\beta g}$	$E_{\frac{3}{2}}$	$E_{\frac{1}{2}u}$	E_2	I_{β}	T_1+T_2	$2T_u$	$E_{1\alpha}+E_{2\alpha}+E_{3\alpha}$	I_{β}	$2T_u$	$E_{1\alpha}+E_{2\alpha}+E_{3\alpha}$	$G_{3\alpha\beta}$	$2G_{\frac{3}{2}u}$	$G'_{\alpha}+G_{\alpha}$
$E'''_{\alpha\beta u}$	$E_{\frac{1}{2}}$	$E_{\frac{1}{2}u}$	E_1	$G_{1\alpha\beta}$	$G_{\frac{1}{2}}$	$2E_{\frac{1}{2}u}$	$E_{1\alpha}+E_{3\alpha}$	$G_{1\alpha\beta}$	$E_{\frac{1}{2}u}$	$E_{1\alpha}+E_{3\alpha}$			
$G_{\alpha\beta g}$	$G_{\frac{3}{2}}$	$G_{\frac{3}{2}u}$	$A_1+A_2+E_2$	$G_{2\alpha\beta}$	$G_{\frac{3}{2}}$	$G_{\frac{3}{2}u}$	$E_{1\alpha}+E_{2\alpha}$	$G_{2\alpha\beta}$	$G_{\frac{3}{2}u}$	$E_{2\alpha}+E_{3\alpha}$			
$G_{\alpha\beta u}$	$G_{\frac{3}{2}}$	$G_{\frac{3}{2}u}$	$B_1+B_2+E_1$	$G_{3\alpha\beta}$	$G_{\frac{3}{2}}$	$G_{\frac{3}{2}u}$	$E_{2\alpha}+E_{3\alpha}$	$G_{3\alpha\beta}$	$G_{\frac{3}{2}u}$	$E_{1\alpha}+E_{2\alpha}$			

Table 5. Correlation of the irreducible representations of the representation groups of the octahedral groups with those of their maximal subgroups. Entries for the subgroups $\mathcal{R}_1(T_d)$ and $\mathcal{R}_2(T_d)$ are identical with those for the isomorphic groups $\mathcal{R}_1(O)$ and $\mathcal{R}_2(O)$.

$R(I)$	$R(T)$	D_5	D_3
A	A	A_1	A_1
T_1	T	A_2+E_1	A_2+E
T_2	T	A_2+E_2	A_2+E
G	A+T	E_1+E_2	A_1+A_2+E
H	E+T	$A_1+E_1+E_2$	A_1+2E
$E_{\frac{1}{2}}$	$E_{\frac{1}{2}}$	E_2	E
$E_{\frac{3}{2}}$	$E_{\frac{1}{2}}$	E_1	E
$G_{\frac{3}{2}}$	$G_{\frac{3}{2}}$	E_1+E_2	A_1+A_2+E
$I_{\frac{5}{2}}$	$E_{\frac{1}{2}}+G_{\frac{3}{2}}$	$A_1+A_2+E_1+E_2$	A_1+A_2+2E

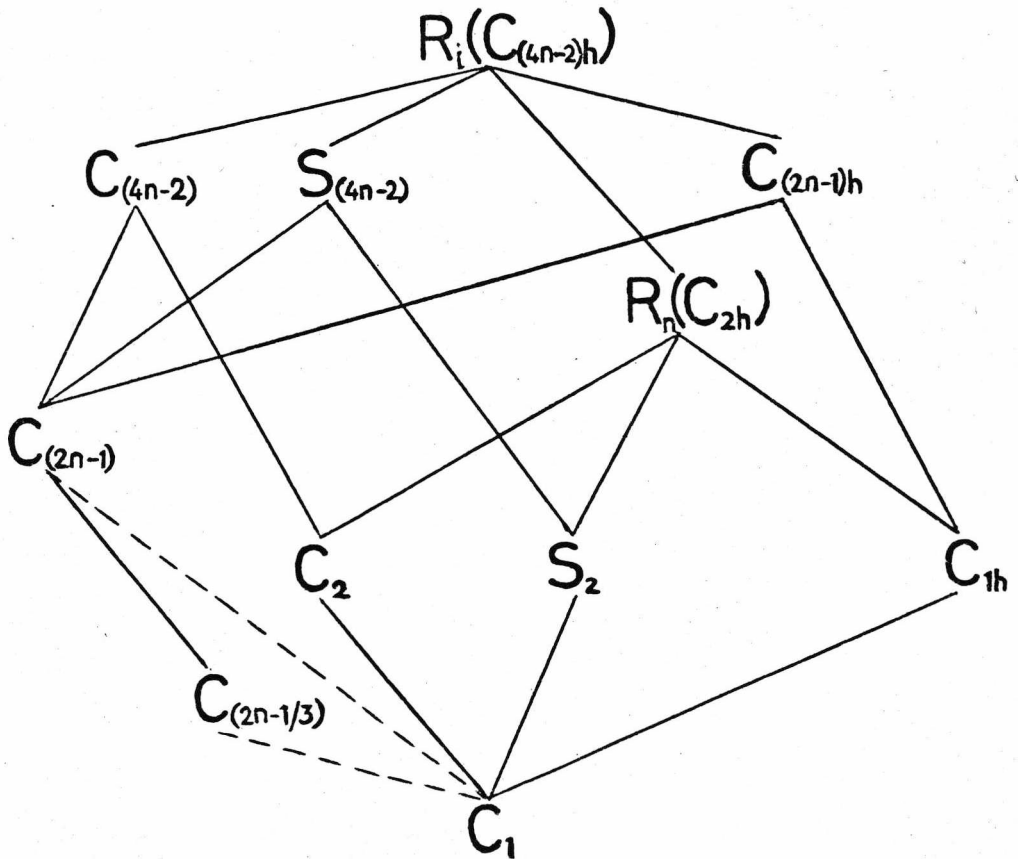
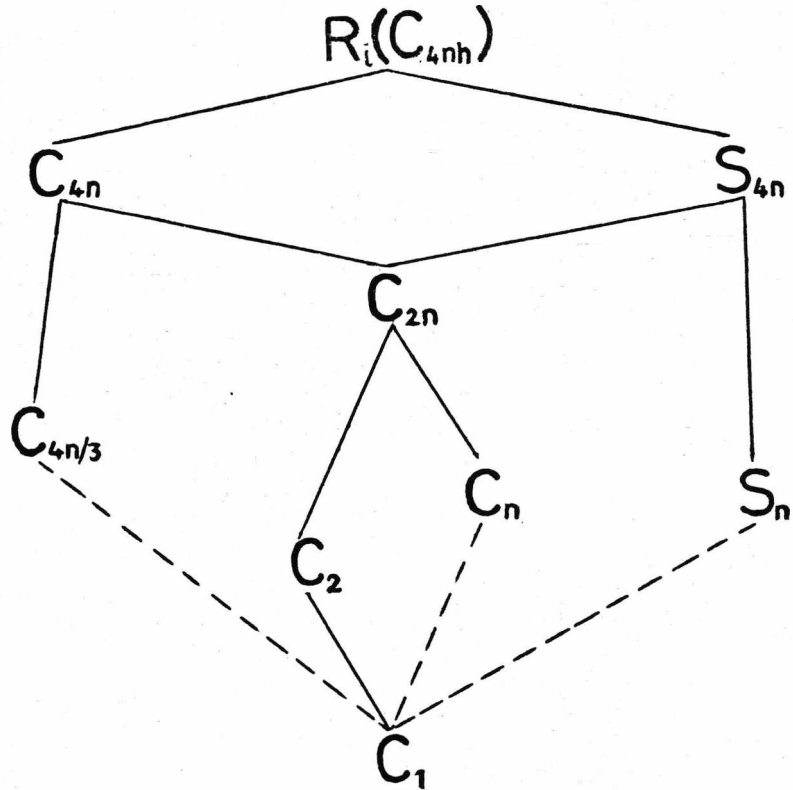
$R_1(I_h)$	$R(I)$	$R_1(T_h)$	$R_2(I_h)$	$R(I)$	$R_2(T_h)$
A_g	A	A_g	A_g	A	A_g
A_u	A	A_u	A_u	A	A_u
T_{1g}	T_1	T_g	T_{1g}	T_1	T_g
T_{1u}	T_1	T_u	T_{1u}	T_1	T_u
T_{2g}	T_2	T_g	T_{2g}	T_2	T_g
T_{2u}	T_2	T_u	T_{2u}	T_2	T_u
G_g	G	A_g+T_g	G_g	G	A_g+T_g
G_u	G	A_u+T_u	G_u	G	A_u+T_u
H_g	H	E_g+T_g	H_g	H	E_g+T_g
H_u	H	E_u+T_u	H_u	H	E_u+T_u
$E_{\frac{1}{2}g}$	$E_{\frac{1}{2}}$	$E_{\frac{1}{2}g}$	$G_{\frac{1}{2}g}$	$2E_{\frac{1}{2}}$	G_g
$E_{\frac{1}{2}u}$	$E_{\frac{1}{2}}$	$E_{\frac{1}{2}u}$	$G_{\frac{1}{2}u}$	$2E_{\frac{1}{2}}$	G_u
$E_{\frac{3}{2}g}$	$E_{\frac{3}{2}}$	$E_{\frac{3}{2}g}$	K_g	$2G_{\frac{3}{2}}$	$G'_g+G''_g$
$E_{\frac{3}{2}u}$	$E_{\frac{3}{2}}$	$E_{\frac{3}{2}u}$	O_u	$2I_{\frac{5}{2}}$	$G'_u+G''_u$
$G_{\frac{3}{2}g}$	$G_{\frac{3}{2}}$	$G_{\frac{3}{2}g}$			
$G_{\frac{3}{2}u}$	$G_{\frac{3}{2}}$	$G_{\frac{3}{2}u}$			
$I_{\frac{5}{2}g}$	$I_{\frac{5}{2}}$	$E_{\frac{1}{2}g}+G_{\frac{3}{2}g}$			
$I_{\frac{5}{2}u}$	$I_{\frac{5}{2}}$	$E_{\frac{1}{2}u}+G_{\frac{3}{2}u}$			

Table 6. Correlation of the irreducible representations of the representation groups of the icosahedral groups with those of their maximal subgroups.

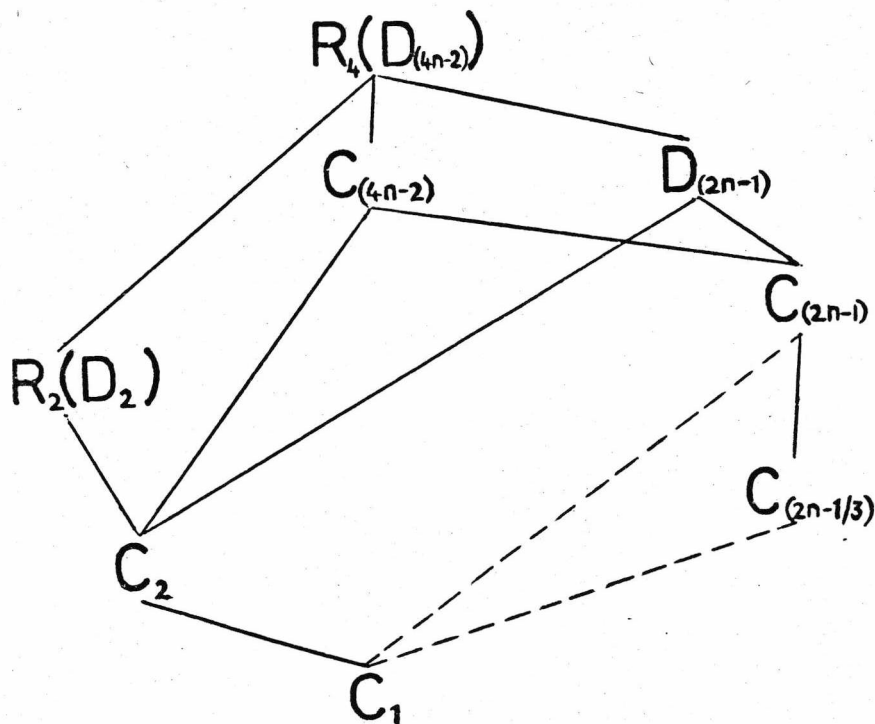
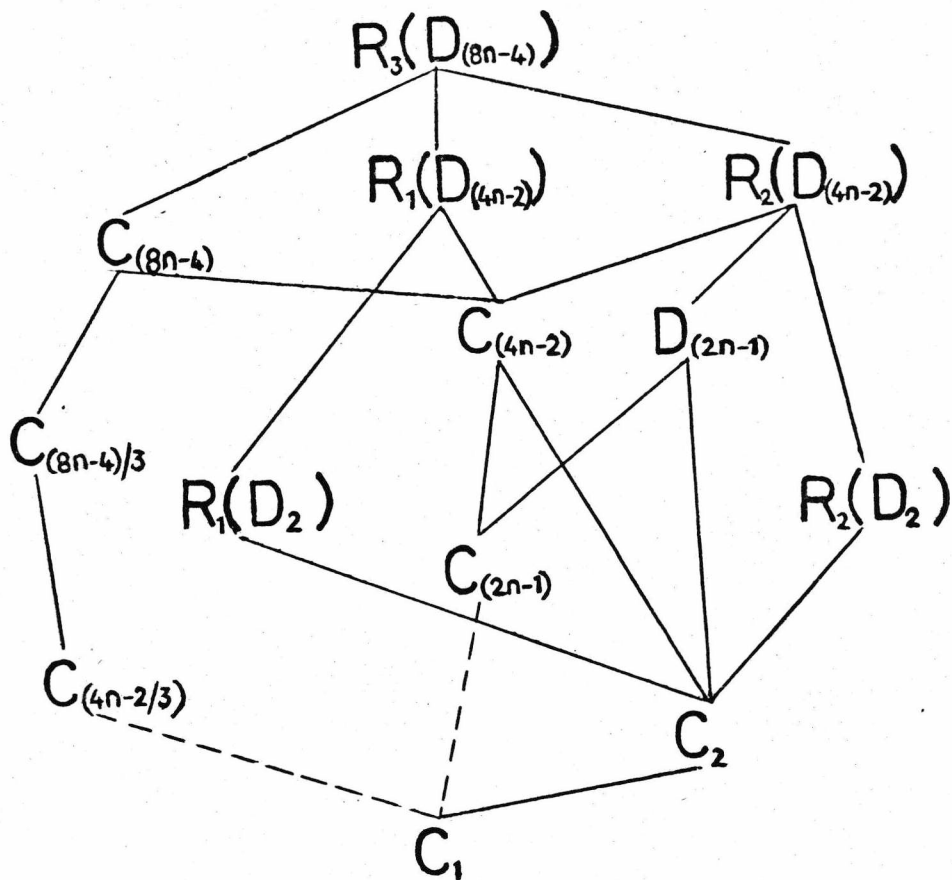
$R_1(K_h)$	$R_1(I_h)$	$R_2(K_h)$	$R_2(I_h)$
D_{0g}	A_g	D_{0g}	A_g
D_{0u}	A_u	D_{0u}	A_u
D_{1g}	T_{1g}	D_{1g}	T_g
D_{1u}	T_{1u}	D_{1u}	T_u
D_{2g}	H_g	D_{2g}	H_g
D_{2u}	H_u	D_{2u}	H_u
D_{3g}	$T_{2g}+G_g$	D_{3g}	$T_{2g}+G_g$
D_{3u}	$T_{2u}+G_u$	D_{3u}	$T_{2u}+G_u$
.....
$D_{\frac{1}{2}g}$	$E_{\frac{1}{2}g}$	$D_{\frac{1}{2}g}$	G_{1g}
$D_{\frac{1}{2}u}$	$E_{\frac{1}{2}u}$	$D_{\frac{1}{2}u}$	K_u
$D_{\frac{3}{2}g}$	$G_{\frac{3}{2}g}$	$D_{\frac{3}{2}g}$	O_g
$D_{\frac{3}{2}u}$	$G_{\frac{3}{2}u}$	$D_{\frac{3}{2}u}$	$G_{2u}+O_u$
$D_{\frac{5}{2}g}$	$I_{\frac{5}{2}g}$
$D_{\frac{5}{2}u}$	$I_{\frac{5}{2}u}$
$D_{\frac{7}{2}g}$	$E_{\frac{1}{2}g}+I_{\frac{5}{2}g}$
$D_{\frac{7}{2}u}$	$E_{\frac{1}{2}u}+I_{\frac{5}{2}u}$

Table 7. Correlation of the irreducible representations of the representation groups of the spherical rotation-reflection group K_h with those of its maximal subgroups.

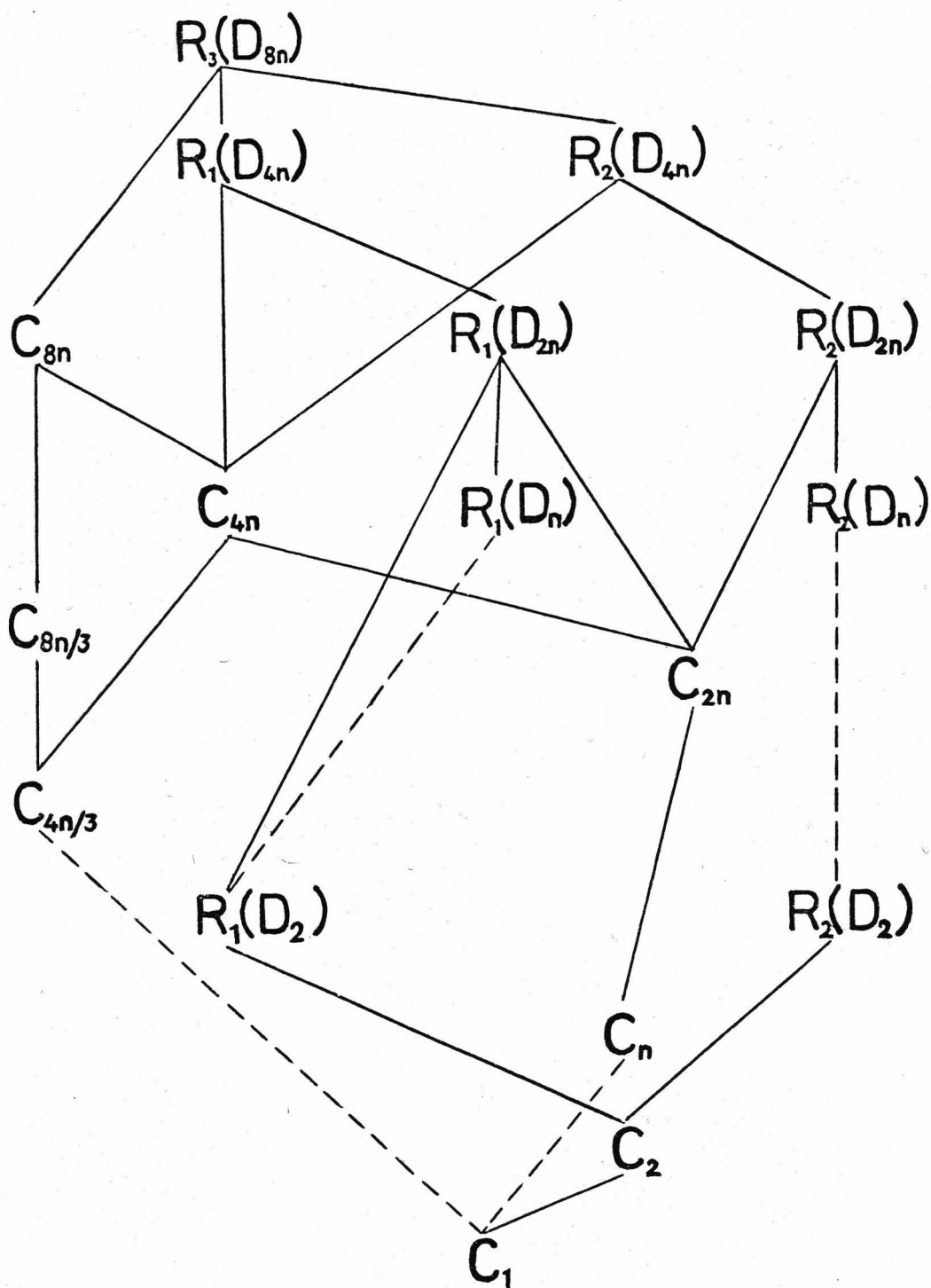
4.I.2 Subgroups of the Representation Groups



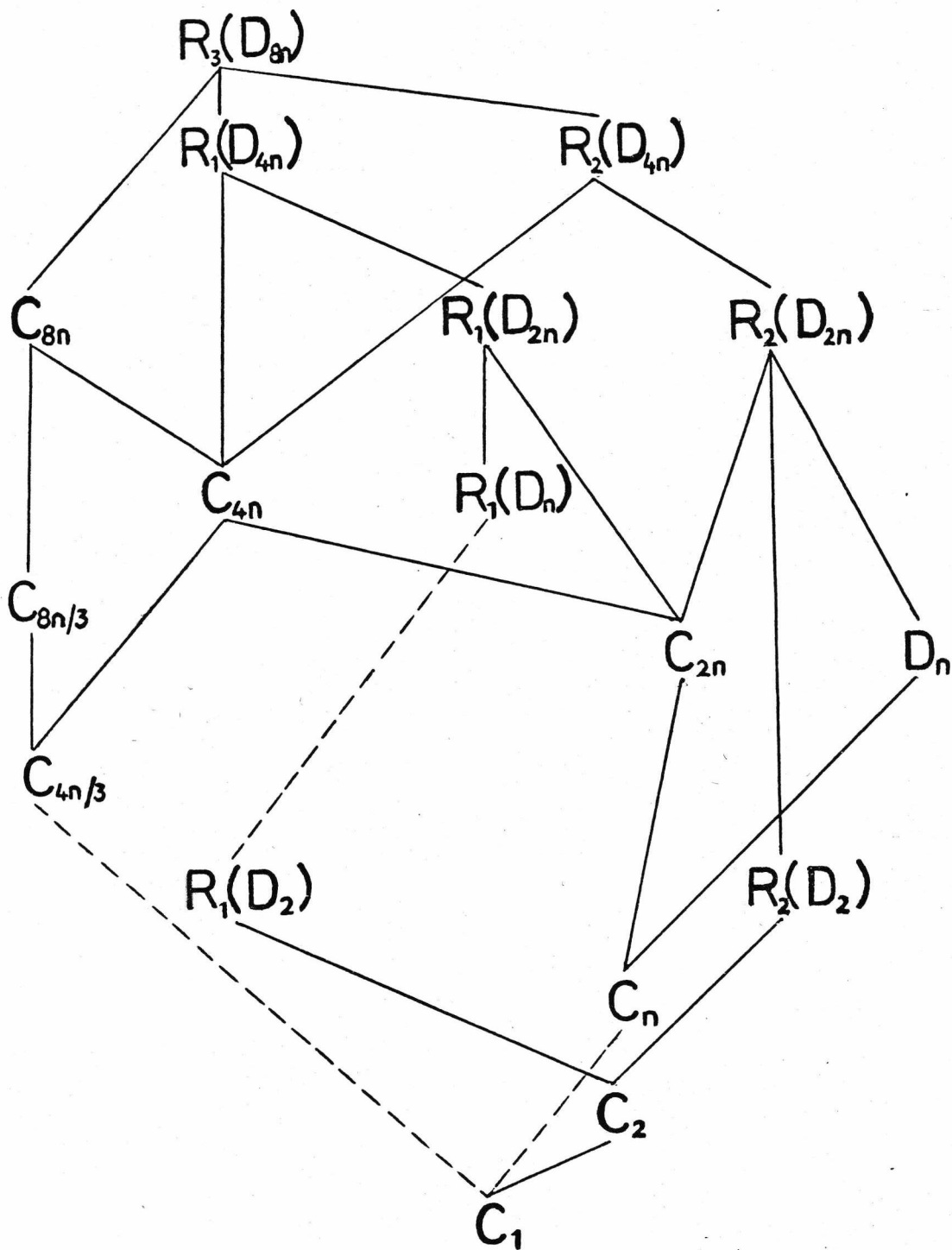
SUBGROUPS OF $R_i(C_{4nh})$ & $R_i(C_{(4n-2)h})$, $i=1,2$



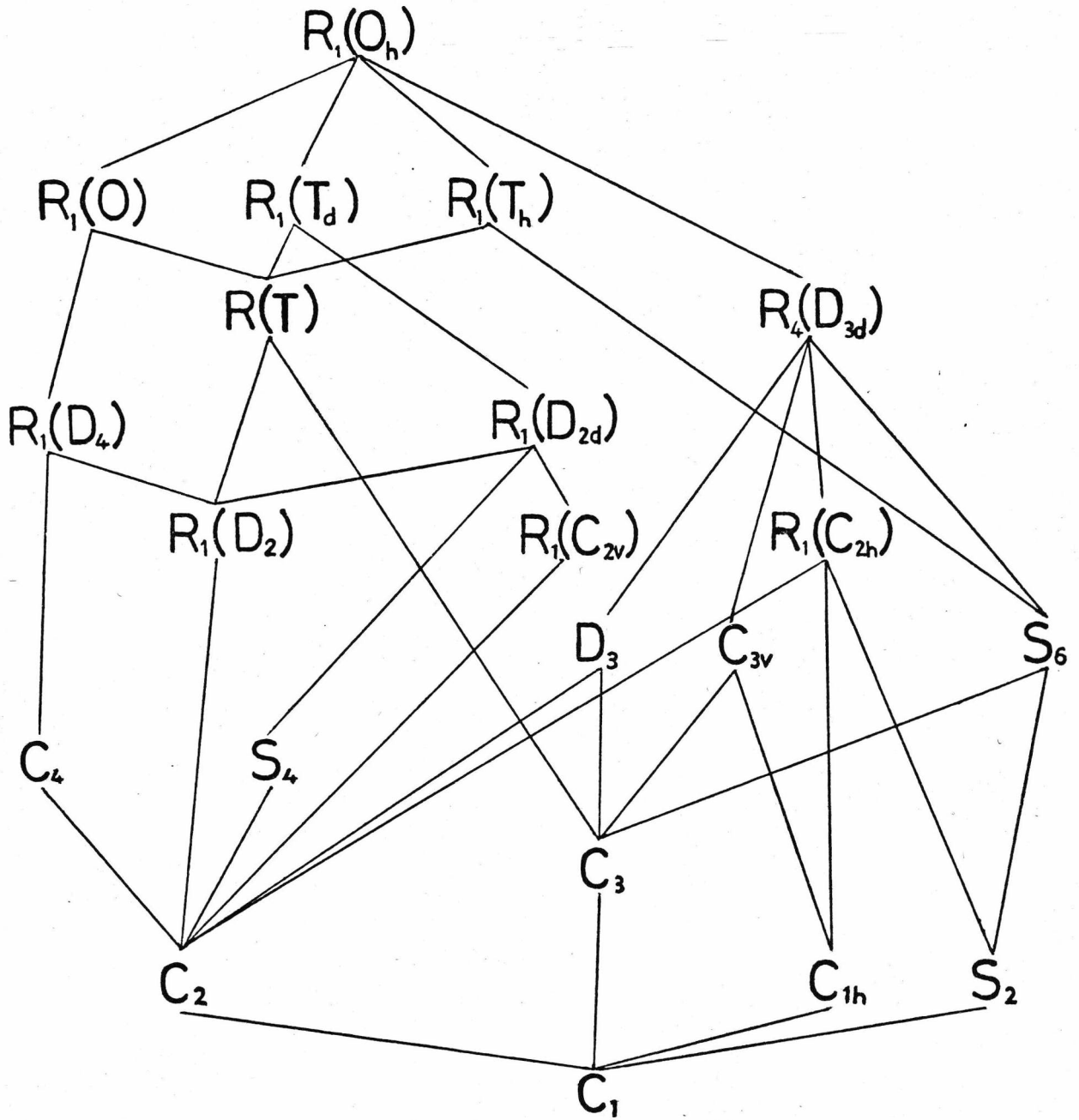
SUBGROUPS OF $R_3(D_{8n-4})$ & $R_4(D_{4n-2})$



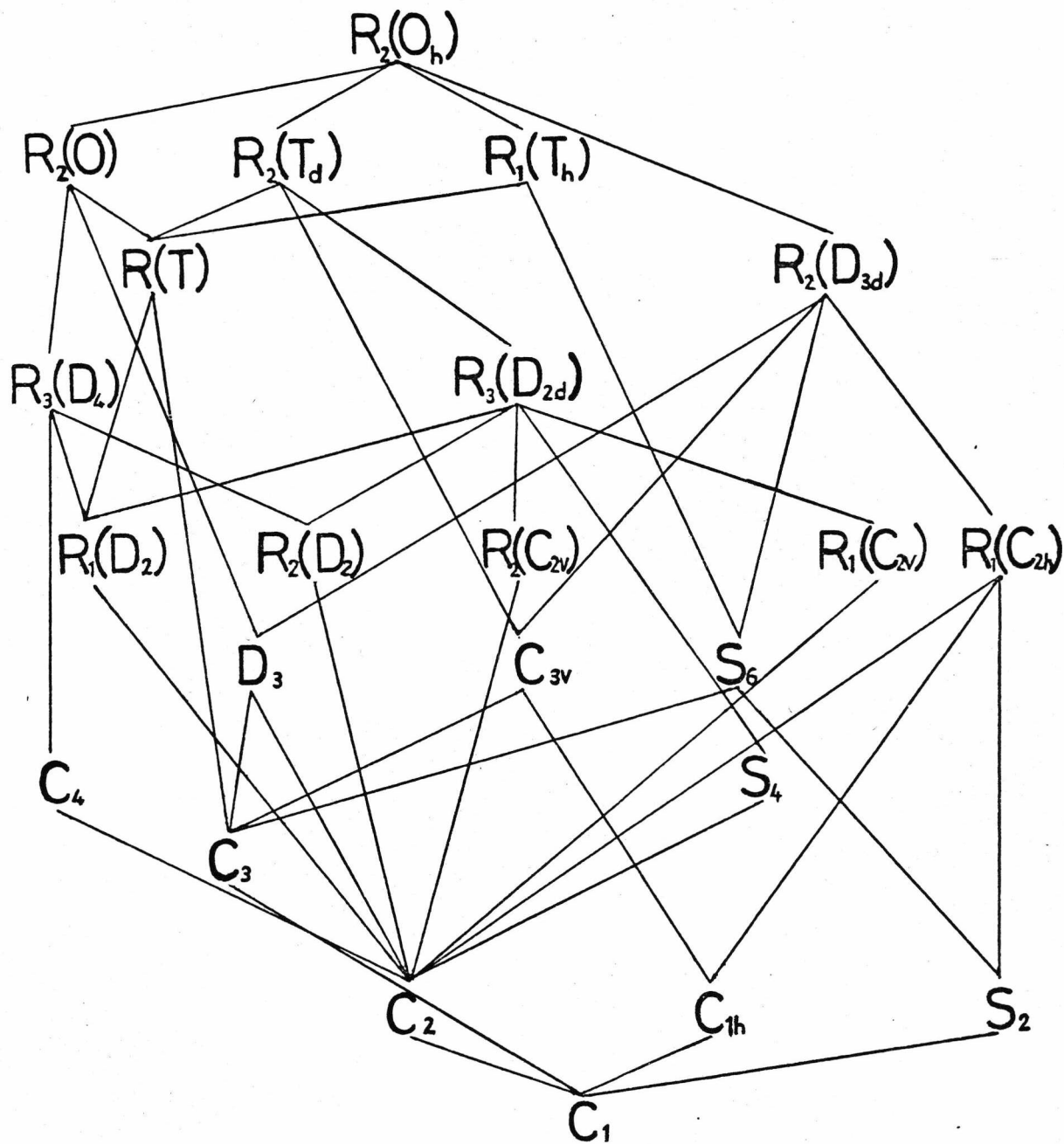
SUBGROUPS OF $R_3(D_{8n})$, n even



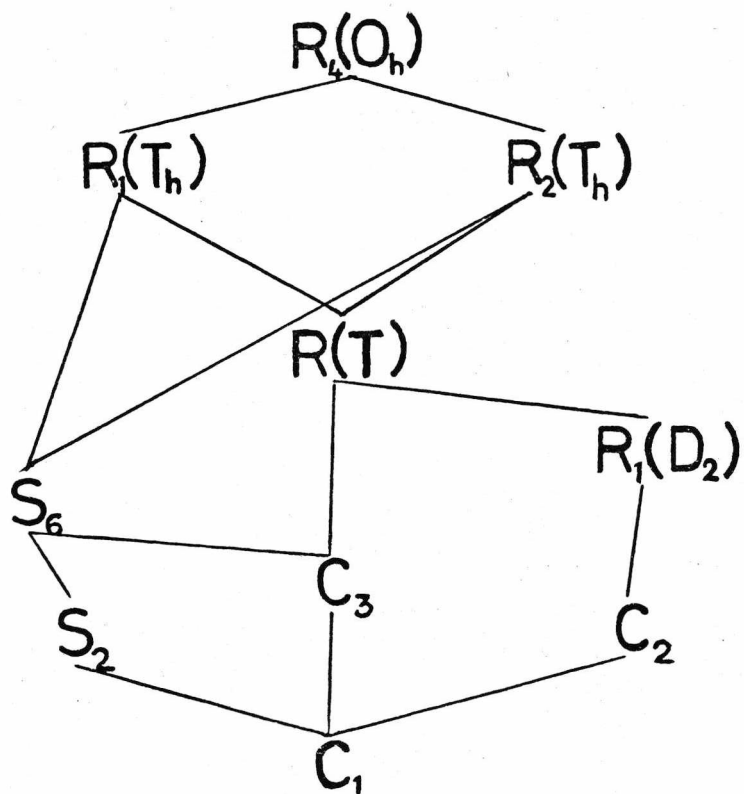
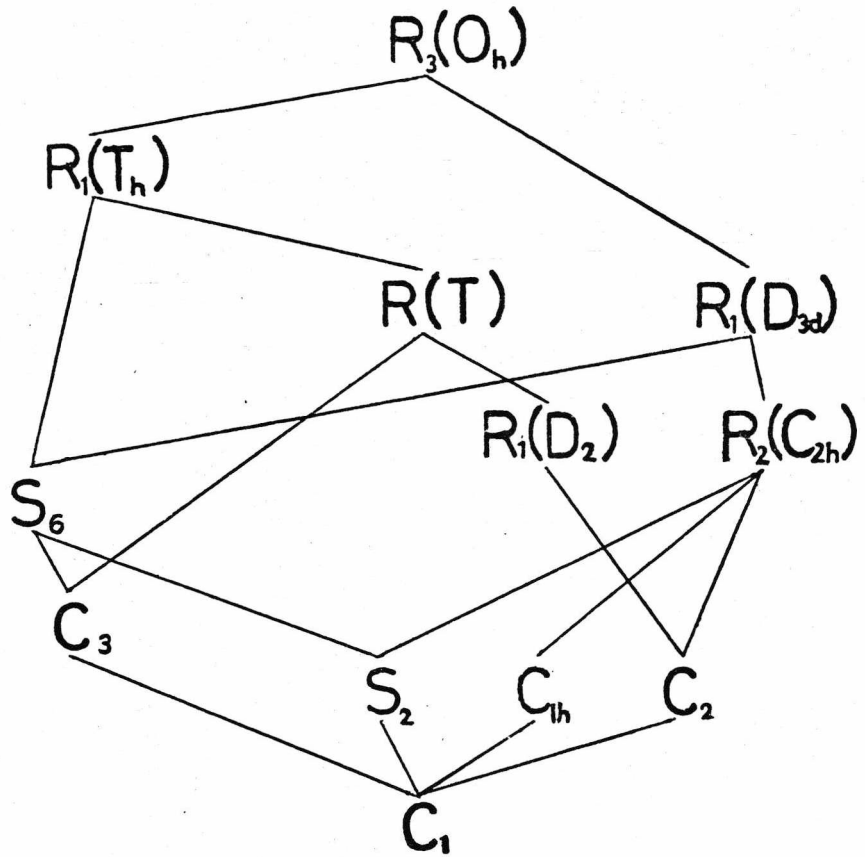
SUBGROUPS OF $R_3(D_{8n})$, n odd



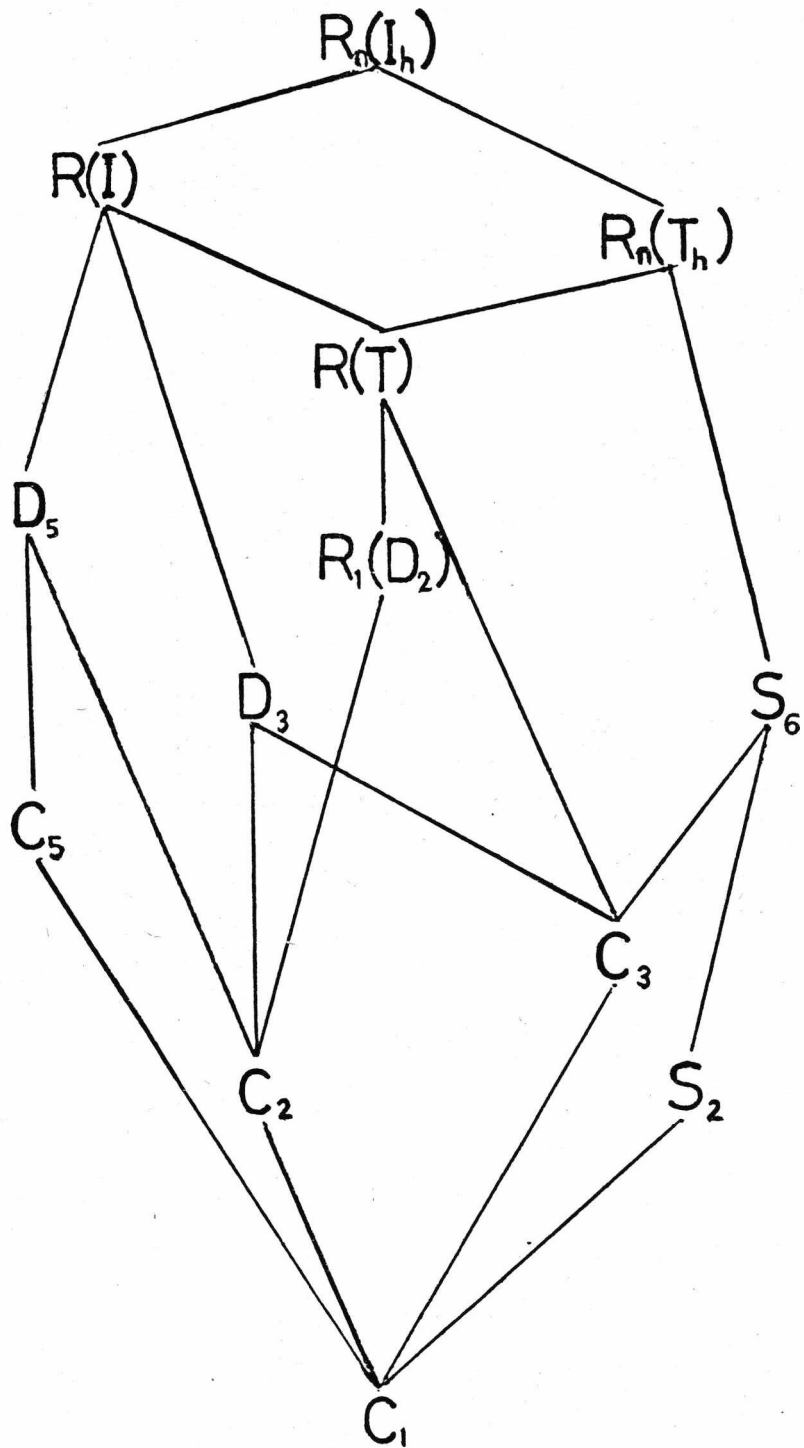
SUBGROUPS OF $R_1(O_h)$



SUBGROUPS OF $R_2(O_h)$



SUBGROUPS OF $R_3(O_h)$ & $R_4(O_h)$



SUBGROUPS OF $R_n(I_h), n=1, 2$

4.2 THE SYMMETRIZED POWERS OF PROJECTIVE REPRESENTATIONS

The concept of symmetrized and antisymmetrized powers of group representations is based on the fact that the wave function of a set of identical particles must be either symmetric or antisymmetric with respect to the interchange of any pair of these identical particles. The total wave function being symmetric for bosons and antisymmetric for fermions. The cases of particular physical interest are those of the symmetrized squares and cubes. The symmetric square is used in the determination of the second excited state of a degenerate vibrational mode, the antisymmetric square in determining expectation values for an imaginary operator. The symmetrized cubes are needed in the Landau-Lifshitz (⁴⁴) theory of second-order phase transitions.

The direct product of projective representations has been considered by Rudra (₃₄) and corrected by Harter (₄₃). However, the resulting formulae are unwieldy because by not involving the actual representation groups they require the knowledge of the large numbers of factor systems of the projective representations and the formation of lengthy products of these.

The use of the standard formulae for vector representations in the representation group, however, enables the calculation to be performed for projective representations without reference to factor systems. Further, there are no complications or need for special theories in the calculation of the symmetrized powers of projective representations. Hence the following standard formulae have been used, where $\chi(g)$ is the character of the representation under the element g . The notation of Tisza (₄₅) has been used where A' symmetric square, A'' antisymmetric square, A_1 symmetric cube, A_2 determinantally-antisymmetric cube and ϵ the permutationally-degenerate part of the cube.

$$A' : \frac{1}{2} \{ \chi^2(g) + \chi(g^2) \}$$

$$A'' : \frac{1}{2} \{ \chi^2(g) - \chi(g^2) \}$$

$$A_1 : \frac{1}{6} \{ \chi^3(g) + 2\chi(g^3) + 3\chi(g)\chi(g^2) \}$$

$$A_2 : \frac{1}{6} \{ \chi^3(g) + 2\chi(g^3) - 3\chi(g)\chi(g^2) \}$$

$$\epsilon : \frac{2}{3} \{ \chi^3(g) - \chi(g^3) \}$$

The results are summarized in the following tables. The symmetrized powers of the vector representations of the representation groups are the same as those for the corresponding point groups and may be found in the papers of Jahn and Teller (24) and Boyle (46).

The fact that the powers of any representation of a group must be symmetrizable provides convincing proof of errors in the underived tables of projective representations published by Janssen (37). By deducing the representation group from the projective representations published one can by comparison with our tables deduce the characters for those elements of the representation group which do not map onto G and hence perform a rigorous symmetrization - usually the symmetrization of the square is sufficient to reveal discrepancy. In this way the characters of magnitude 2i in the projective representations Γ_{13} and Γ_{21} of D_{2h} were found to be actually 2 while the 2 in Γ_{15} should be 2i. Döring's (33) and Hurley's (35) projective representations for D_{2h} were similarly wrong since their projective representations only contain real characters.

It will be noticed from the tables that the symmetrized powers of projective representations differ considerably according to the representation group chosen. However, in physical problems such as those to be discussed in the next chapter, there will always be one choice for which the set of projective characters is physically relevant without modification. Hence by identifying this choice the following tables can be used to solve any given physical problem requiring symmetrized squares or cubes.

$\mathcal{R}_1(C_{4nh})$

$$\begin{aligned} E_{n\alpha}^2 &= \{A_u + B_g + B_u | A'\} + \{A_g | A''\} \\ E_{2n\alpha}^2 &= \{A_g + A_u + B_u | A'\} + \{B_g | A''\} \\ G_{l\alpha}^2 &= \{A_g + A_u + B_g + B_u + E_{|2n-2l-1|u} + E_{\{14n-2l-1\} \bmod 2n} g + \\ &\quad + E_{\{14n-2l-1\} \bmod 2n} u | A'\} + \{A_g + A_u + B_g + B_u + \\ &\quad + E_{|2n-2l-1|g} | A''\} \end{aligned}$$

$\mathcal{R}_2(C_{4nh})$

$$\begin{aligned} G_{l\alpha}^2 &= \{A_g + A_u + B_g + B_u + E_{(2l-1)g} + E_{(2l-1)u} + E_{|2n-2l+1|g} | A'\} + \\ &\quad + \{A_g + A_u + B_g + B_u + E_{|2n-2l+1|u} | A''\} \end{aligned}$$

$\mathcal{R}_1(C_{(4n-2)h})$

$$\begin{aligned} E_{(2n-1)\alpha}^2 &= \{A_g + A_u + B_g | A'\} + \{B_u | A''\} \\ G_{l\alpha}^2 &= \{A_g + A_u + B_g + B_u + E_{|2n-2l-2|g} + E_{\{14n-2l-3\} \bmod (2n-1)} g + \\ &\quad + E_{\{14n-2l-3\} \bmod (2n-1)} u | A'\} + \{A_g + A_u + B_g + B_u + \\ &\quad + E_{|2n-2l-2|u} | A''\} \end{aligned}$$

$\mathcal{R}_2(C_{(4n-2)h})$

$$\begin{aligned} E_{\alpha}^2 &= \{A_u + B_g + B_u | A'\} + \{A_g | A''\} \\ G_{l\alpha}^2 &= \{A_g + A_u + B_g + B_u + E_{(2l-1)g} + E_{(2l-1)u} + E_{|2n-2l|u} | A'\} + \\ &\quad + \{A_g + A_u + B_g + B_u + E_{|2n-2l|g} | A''\} \end{aligned}$$

$\mathcal{R}_1(D_{4n}), \mathcal{R}_1(C_{4nv}), \mathcal{R}_1(D_{2nd})$

$$E_{l\alpha}^2 = \{A_2 + E_{2n-|2n-(2l-1) \bmod 2n|} | A'\} + \{A_1 | A''\}$$

$\mathcal{R}_2(D_{4n}), \mathcal{R}_2(C_{4nv}), \mathcal{R}_2(D_{2nd})$

$$E_{l\alpha}^2 = \{A_1 + E_{2n-|2n-(2l-1) \bmod 2n|} | A'\} + \{A_2 | A''\}$$

$\mathcal{R}_3(D_{4n}), \mathcal{R}_3(C_{4nv}), \mathcal{R}_3(D_{2nd})$

$$\begin{aligned} G_{l\alpha}^2 &= \{A_1 + A_2 + 2B_1 + E_{|2n-2l+1| \bmod 2n} + 2E_{\{4n-2l+1\} \bmod 2n} | A'\} + \\ &\quad + \{A_1 + A_2 + 2B_2 + E_{|2n-2l+1| \bmod 2n} | A''\} \end{aligned}$$

$\mathcal{R}_1(D_{4n-2}), \mathcal{R}_1(C_{(4n-2)v})$,

$$E_{l\alpha}^2 (l \neq n) = \{A_2 + E_{2n-1-|2n-1-(2l-1) \bmod (2n-1)|} | A'\} + \{A_1 | A''\}$$

$\mathcal{R}_1(D_{(2n-1)d}), \mathcal{R}_1(D_{(2n-1)h})$

$$E_{n\alpha}^2 = \{A_2 + B_1 + B_2 | A'\} + \{A_1 | A''\}$$

$\mathcal{R}_2(D_{4n-2}), \mathcal{R}_2(C_{(4n-2)v})$,

$$E_{l\alpha}^2 (l \neq n) = \{A_1 + E_{2n-1-|2n-1-(2l-1) \bmod (2n-1)|} | A'\} + \{A_2 | A''\}$$

$\mathcal{R}_2(D_{(2n-1)d}), \mathcal{R}_2(D_{(2n-1)h})$

$$E_{n\alpha}^2 = \{A_1 + B_1 + B_2 | A'\} + \{A_2 | A''\}$$

$$\begin{aligned}
 & R_3(D_{4n-2}), R_3(C_{(4n-2)v}), E_\alpha^2 = \{A_1 + A_2 + B_2 | A'\} + \{B_1 | A''\} \\
 & R_3(D_{(2n-1)d}), R_3(D_{(2n-1)h}) G_{\alpha}^2 = \{A_1 + A_2 + 2B_2 + E_{|2n-4l-1| \bmod (2n-1)} + 2E_{|2n-4n-8l-2| \bmod (4n-2)} | A'\} + \\
 & \quad + \{A_1 + A_2 + 2B_1 + E_{|2n-4l-1| \bmod (2n-1)} | A''\}
 \end{aligned}$$

$R_1(D_{4nh})$

$$E_{\alpha}^2 = \{A_{1g} + E_{\{2n-|2n-(2l+1)| \bmod 2n\}} | A'\} + \{A_{2g} | A''\}$$

$$E_{1\beta}^2 = E_{2\beta}^2 = \{A_{1g} + A_{1u} + A_{2g} | A'\} + \{A_{2u} | A''\}$$

$$\begin{aligned}
 G_{\alpha\beta}^2 = \{ & A_{1g} + 2A_{1u} + A_{2g} + 3E_{\{(2n-|2n-2l|) \bmod 2n\}u} | A'\} + \{A_{1g} + \\
 & + A_{2g} + 2A_{2u} + E_{\{(2n-|2n-2l|) \bmod 2n\}u} | A''\}
 \end{aligned}$$

$$E_{1\gamma}^2 = E_{2\gamma}^2 = \{A_{1g} + A_{2u} + B_{2u} | A'\} + \{B_{1g} | A''\}$$

$$\begin{aligned}
 G_{\gamma}^2 = \{ & A_{1g} + A_{1u} + 2A_{2u} + B_{1g} + B_{1u} + 2B_{2g} + 2B_{2u} | A'\} + \{A_{1g} + A_{1u} + \\
 & + 2A_{2g} + B_{1g} + B_{1u} | A''\}
 \end{aligned}$$

$$\begin{aligned}
 G_{\gamma\delta}^2 = \{ & A_{1g} + A_{2u} + B_{2g} + B_{2u} + E_{2lg} + E_{2lu} + E_{|2n-2l|u} | A'\} + \{A_{1u} + \\
 & + A_{2g} + B_{1g} + B_{1u} + E_{|2n-2l|g} | A''\}
 \end{aligned}$$

$$\begin{aligned}
 G_{\alpha\beta}^2 = \{ & A_{1g} + 2A_{1u} + A_{2g} + E_{\{(2n-|2n-2l+1|) \bmod 2n\}g} + \\
 & + 2E_{\{(2n-|2n-2l+1|) \bmod 2n\}u} | A'\} + \{A_{1g} + A_{2g} + 2A_{2u} + \\
 & + E_{\{(2n-|2n-2l+1|) \bmod 2n\}g} | A''\}
 \end{aligned}$$

$$\begin{aligned}
 G_{\alpha\gamma}^2 \text{ (l odd)} = \{ & A_{1g} + A_{2u} + B_{2g} + B_{2u} + 2E_{lu} + E_{|2n-l|u} | A'\} + \\
 & + \{A_{1u} + A_{2g} + B_{1g} + B_{1u} + E_{|2n-l|u} | A''\}
 \end{aligned}$$

$$\begin{aligned}
 G_{\alpha\gamma}^2 \text{ (l even)} = \{ & A_{1g} + A_{2u} + B_{2g} + B_{2u} + 2E_{lg} + E_{|2n-l|g} | A'\} + \\
 & + \{A_{1u} + A_{2g} + B_{1g} + B_{1u} + E_{|2n-l|g} | A''\}
 \end{aligned}$$

$$E_{1\delta\beta}^2 = E_{2\delta\beta}^2 = \{A_{1u} + B_{2g} + B_{2u} | A'\} + \{A_{1g} | A''\}$$

$$\begin{aligned}
 G_{\gamma\beta}^2 = \{ & A_{1g} + 2A_{1u} + 2A_{2g} + A_{2u} + B_{1u} + B_{2g} + 2B_{2u} | A'\} + \{A_{1g} + A_{2u} + \\
 & + 2B_{1g} + B_{1u} + B_{2g} | A''\}
 \end{aligned}$$

$$\begin{aligned}
 G_{\gamma\beta}^2 = \{ & A_{1u} + A_{2g} + B_{2g} + B_{2u} + 2E_{2lg} + E_{|2n-2l|g} | A'\} + \{A_{1g} + A_{2u} + \\
 & + B_{1g} + B_{1u} + E_{|2n-2l|g} | A''\}
 \end{aligned}$$

$$\begin{aligned}
 G_{\alpha\beta\delta}^2 \text{ (l odd)} = \{ & A_{1u} + A_{2g} + B_{2g} + B_{2u} + 2E_{lu} + E_{|2n-l|u} | A'\} + \\
 & + \{A_{1g} + A_{2u} + B_{1g} + B_{1u} + E_{|2n-l|u} | A''\}
 \end{aligned}$$

$$\begin{aligned}
 G_{\alpha\beta\delta}^2 \text{ (l even)} = \{ & A_{1u} + A_{2g} + B_{2g} + B_{2u} + 2E_{lg} + E_{|2n-l|g} | A'\} + \\
 & + \{A_{1g} + A_{2u} + B_{1g} + B_{1u} + E_{|2n-l|g} | A''\}
 \end{aligned}$$

$\mathcal{R}_2(D_{4nh})$

$$G_{\lambda\alpha}^2 = \{A_{1g} + A_{1u} + B_{1g} + B_{2u} + E_{12n-2l+1g} + 2E_{12n-12n-2l+1} B_g |A'\} + \{A_{2g} + A_{2u} + B_{2g} + B_{2u} + E_{12n-2l+1g} |A''\}$$

$$E_{1\beta}^2 = E_{2\beta}^2 = \{A_{1g} + A_{1u} + A_{2g} |A'\} + \{A_{2u} |A''\}$$

$$G_{\lambda\beta}^2 = \{A_{1g} + 2A_{1u} + A_{2g} + 2B_{1g} + B_{1u} + 2B_{2g} + B_{2u} |A'\} + \{A_{1g} + A_{2g} + 2A_{2u} + B_{1u} + B_{2u} |A''\}$$

$$E_{1\delta}^2 = E_{2\delta}^2 = \{A_{1g} + A_{2u} + B_{2u} |A'\} + \{B_{1g} |A''\}$$

$$G_{\gamma}^2 = \{A_{1g} + A_{1u} + 2A_{2u} + B_{1g} + B_{1u} + 2B_{2g} + 2B_{2u} |A'\} + \{A_{1g} + A_{1u} + 2A_{2g} + B_{1g} + B_{1u} |A''\}$$

$$G_{(1/2n+1/2)\delta}^2 = \{2A_{1g} + A_{2g} + A_{2u} + 2B_{1u} + B_{2g} + B_{2u} |A'\} + \{A_{1g} + A_{1u} + 2A_{2g} + B_{1g} + B_{1u} |A''\}$$

$$G_{\lambda\delta}^2 (l \neq \frac{1}{2}n + \frac{1}{2}) = \{A_{1g} + A_{2u} + B_{2g} + B_{2u} + E_{12n-4l+2} g + 2E_{12n+4l-2} u |A'\} + \{A_{1u} + A_{2g} + B_{1g} + B_{1u} + E_{12n-4l+2} g |A''\}$$

$$G_{\lambda\alpha\beta}^2 = \{A_{1g} + A_{2g} + 2B_{1u} + 2E_{12n-12n-2l+1} g + E_{12n-2l+1} u |A'\} + \{A_{1g} + A_{2g} + 2B_{2u} + E_{12n-2l+1} u |A''\}$$

$$G_{\lambda\alpha\delta}^2 = \{A_{2g} + A_{2u} + B_{1g} + B_{2u} + E_{12n-2l+1} g + 2E_{12n-12n-2l+1} g |A'\} + \{A_{1g} + A_{1u} + B_{1u} + B_{2g} + E_{12n-2l+1} g |A''\}$$

$$E_{1\beta\delta}^2 = E_{2\beta\delta}^2 = \{A_{1u} + B_{2g} + B_{2u} |A'\} + \{A_{1g} |A''\}$$

$$G_{\beta\delta}^2 = \{A_{1g} + 2A_{1u} + 2A_{2g} + A_{2u} + B_{1u} + B_{2g} + 2B_{2u} |A'\} + \{A_{1g} + A_{2u} + 2B_{1g} + B_{1u} + B_{2g} |A''\}$$

$$G_{(1/2n+1/2)\beta\delta}^2 = \{A_{1g} + A_{1u} + 2A_{2g} + B_{1g} + 2B_{2g} + B_{2u} |A'\} + \{2A_{1g} + A_{2g} + A_{2u} + B_{1g} + B_{1u} |A''\}$$

$$G_{\lambda\beta\delta}^2 (l \neq \frac{1}{2}n + \frac{1}{2}) = \{A_{1u} + A_{2g} + B_{2g} + B_{2u} + E_{12n-4l+2} g + 2E_{12n-12n-4l+2} u |A'\} + \{A_{1g} + A_{2u} + B_{1g} + B_{1u} + E_{12n-4l+2} g |A''\}$$

$$G_{\lambda\alpha\beta\delta}^2 = \{A_{2g} + A_{2u} + B_{1u} + B_{2g} + E_{12n-2l+1} g + 2E_{12n-12n-2l+1} u |A''\} + \{A_{1g} + A_{1u} + B_{1g} + B_{2u} + E_{12n-2l+1} g |A''\}$$

$\mathcal{R}_1(D_{(4n-2)h})$

$$E_{n\alpha}^2 = \{A_{1g} + B_{1u} + B_{2u} |A'\} + \{A_{2g} |A''\}$$

$$E_{\lambda\alpha}^2 (l \neq n) = \{A_{1g} + E_{12n-1-12n-2l} \} \text{mod}(2n-1) u |A'\} + \{A_{2g} |A''\}$$

$$E_{1\beta}^2 = E_{2\beta}^2 = \{A_{1g} + A_{1u} + A_{2g} |A'\} + \{A_{2u} |A''\}$$

$$G_{\lambda\beta}^2 = \{A_{1g} + 2A_{1u} + A_{2g} + 3E_{\{2n-1-|2n-2\ell|\} \bmod (2n-1)u} |A'\} + \{A_{1g} + A_{2g} + 2A_{2u} + E_{\{2n-1-|2n-2\ell|\} \bmod (2n-1)u} |A''\}$$

$$E_{1\beta}^2 = E_{2\beta}^2 = \{A_{1g} + A_{2u} + B_{2u} |A'\} + \{B_{1g} |A''\}$$

$$G_{2\beta}^2 = \{A_{1g} + A_{2u} + B_{2g} + B_{2u} + E_{2\beta g} + E_{|2n-2\ell-1|g} + E_{2\beta u} |A'\} + \{A_{1u} + A_{2g} + B_{1g} + B_{1u} + E_{|2n-2\ell-1|u} |A''\}$$

$$G_{n\beta}^2 = \{A_{1g} + 2A_{1u} + A_{2g} + B_{1g} + 2B_{1u} + B_{2g} + 2B_{2u} |A'\} + \{A_{1g} + A_{2g} + 2A_{2u} + B_{1g} + B_{2g} |A''\}$$

$$G_{\lambda\alpha}^2 (\ell \neq n) = \{A_{1g} + 2A_{1u} + A_{2g} + E_{\{2n-1-|2n-2\ell|\} \bmod (2n-1)g} + 2E_{\{2n-1-|2n-2\ell|\} \bmod (2n-1)u} |A'\} + \{A_{1g} + A_{2g} + 2A_{2u} + E_{\{2n-1-|2n-2\ell|\} \bmod (2n-1)g} |A''\}$$

$$G_{\alpha\beta}^2 = \{A_{1g} + A_{1u} + 2A_{2u} + B_{1g} + B_{1u} + 2B_{2g} + 2B_{2u} |A'\} + \{A_{1g} + A_{1u} + 2A_{2g} + B_{1g} + B_{1u} |A''\}$$

$$G_{\lambda\beta}^2 (\ell \text{ odd}) = \{A_{1g} + A_{2u} + B_{2g} + B_{2u} + 2E_{\lambda u} + 2E_{|2n-\ell-1|g} |A'\} + \{A_{1u} + A_{2g} + B_{1g} + B_{1u} + E_{|2n-\ell-1|g} |A''\}$$

$$G_{1\alpha\beta}^2 (\ell \text{ even}) = \{A_{1g} + A_{2u} + B_{2g} + B_{2u} + 2E_{\lambda g} + 2E_{|2n-\ell-1|u} |A'\} + \{A_{1u} + A_{2g} + B_{1g} + B_{1u} + E_{|2n-\ell-1|u} |A''\}$$

$$G_{\beta\beta}^2 = \{A_{1g} + 2A_{1u} + 2A_{2g} + A_{2u} + B_{1g} + 2B_{2g} + B_{2u} |A'\} + \{A_{1g} + A_{2u} + B_{1g} + 2B_{1u} + B_{2u} |A''\}$$

$$G_{\lambda\beta}^2 = \{A_{1u} + A_{2g} + B_{2g} + B_{2u} + 2E_{\lambda g} + E_{|2n-2\ell-1|u} |A'\} + \{A_{1g} + A_{2u} + B_{1g} + B_{1u} + E_{|2n-2\ell-1|u} |A''\}$$

$$E_{1\alpha\beta}^2 = E_{2\alpha\beta}^2 = \{A_{1u} + B_{2g} + B_{2u} |A'\} + \{A_{1g} |A''\}$$

$$G_{2\alpha\beta}^2 (\ell \text{ odd}) = \{A_{1u} + A_{2g} + B_{2g} + B_{2u} + E_{|2n-\ell-1|g} + 2E_{\lambda u} |A'\} + \{A_{1g} + A_{2u} + B_{1g} + B_{1u} + E_{|2n-\ell-1|g} |A''\}$$

$$G_{\lambda\alpha\beta}^2 (\ell \text{ even}) = \{A_{1u} + A_{2g} + B_{2g} + B_{2u} + E_{|2n-\ell-1|u} + 2E_{\lambda g} |A'\} + \{A_{1g} + A_{2u} + B_{1g} + B_{1u} + E_{|2n-\ell-1|u} |A''\}$$

$R_2(D_{(4n-2)h})$

$$E_{1\alpha}^2 = E_{2\alpha}^2 = \{A_{1g} + B_{1u} + B_{2g} |A'\} + \{A_{2u} |A''\}$$

$$G_{\lambda\alpha}^2 = \{A_{1g} + A_{1u} + B_{1u} + B_{2g} + 2E_{\lambda g} + E_{|2n-\ell-1|u} |A'\} + \{A_{2g} + A_{2u} + B_{1g} + B_{2u} + E_{|2n-\ell-1|u} |A''\}$$

$$\begin{aligned}
 E_{1\beta}^2 &= E_{2\beta}^2 = \{A_{1g} + A_{1u} + B_{2u} | A'\} + \{B_{2g} | A''\} \\
 G_{1\beta}^2 &= \{A_{1g} + A_{1u} + B_{1g} + B_{1u} + E_{|2n-2\ell-1|g} + 2E_{2\ell u} | A'\} + \{A_{2g} + A_{2u} + \\
 &\quad + B_{1u} + B_{2g} + E_{|2n-2\ell-1|g} | A''\} \\
 E_{1\gamma}^2 &= E_{2\gamma}^2 = \{A_{1g} + A_{2g} + A_{2u} | A'\} + \{A_{1u} | A''\} \\
 G_{1\gamma}^2 &= \{A_{1g} + A_{2g} + 2A_{2u} + 2E_{\{2n-1-|2n-2\ell-1|\}g} + E_{\{2n-1-|2n-2\ell-1|\}u} | A'\} + \\
 &\quad + \{A_{1g} + 2A_{2u} + A_{2g} + E_{\{2n-1-|2n-2\ell-1|\}u} | A''\} \\
 G_{n\alpha\beta}^2 &= \{A_{1g} + 2A_{1u} + A_{2g} + 2B_{1g} + B_{1u} + 2B_{2g} + B_{2u} | A'\} + \{A_{1g} + A_{2g} + 2A_{2u} + B_{1u} + B_{2u} | A''\} \\
 G_{l\alpha\beta}^2 (l \neq n) &= \{A_{1g} + 2A_{1u} + A_{2g} + E_{\{2n-1-|2n-2\ell|\}g} + 2E_{\{2n-1-|2n-2\ell|\}u} | A'\} + \\
 &\quad + \{A_{1g} + A_{2g} + 2A_{2u} + E_{\{2n-1-|2n-2\ell|\}u} | A''\} \\
 E_{\alpha\gamma}^2 &= \{A_{1g} + 2A_{2g} + A_{2u} + B_{1g} + 2B_{1u} + 2B_{2g} + B_{2u} | A'\} + \{A_{1g} + 2A_{1u} + \\
 &\quad + A_{2u} + B_{1g} + B_{2u} | A''\} \\
 G_{l\alpha\gamma}^2 &= \{A_{2g} + A_{2u} + B_{1u} + B_{2g} + 2E_{1g} + E_{|2n-\ell-1|u} | A'\} + \{A_{1g} + A_{1u} + \\
 &\quad + B_{1g} + B_{2u} + E_{|2n-\ell-1|u} | A''\} \\
 E_{\beta\gamma}^2 &= \{A_{1g} + A_{1u} + 2A_{2g} + 2A_{2u} + 2B_{1g} + B_{2g} + B_{2u} | A'\} + \{A_{1g} + A_{1u} + \\
 &\quad + 2B_{1u} + B_{2g} + B_{2u} | A''\} \\
 G_{1\beta\gamma}^2 &= \{A_{2g} + A_{2u} + B_{1g} + B_{2u} + 2E_{2\ell u} + E_{|2n-2\ell-1|g} | A'\} + \\
 &\quad + \{A_{1g} + A_{1u} + B_{1u} + B_{2g} + E_{|2n-2\ell-1|g} | A''\} \\
 E_{n\alpha\beta\gamma}^2 &= \{A_{2g} + B_{1g} + B_{2g} | A'\} + \{A_{1g} | A''\} \\
 E_{l\alpha\beta\gamma}^2 (l \neq n) &= \{A_{2g} + E_{\{2n-1-|2n-2\ell|\} \bmod (2n-1)g} | A'\} + \{A_{1g} | A''\}
 \end{aligned}$$

$\mathcal{R}(T)$

$$\begin{aligned}
 E_{\frac{1}{2}}^2 &= \{T | A'\} + \{A | A''\} \\
 G_{\frac{3}{2}}^2 &= \{A + 3T | A'\} + \{A + E + T | A''\}
 \end{aligned}$$

$\mathcal{R}_1(T_h)$

$$\begin{aligned}
 E_{\frac{1}{2}g}^2 &= E_{\frac{1}{2}u}^2 = \{T_g | A'\} + \{A_g | A''\} \\
 G_{\frac{3}{2}g}^2 &= G_{\frac{3}{2}u}^2 = \{A_g + 3T_g | A'\} + \{A_g + E_g + T_g | A''\}
 \end{aligned}$$

$\mathcal{R}_2(T_h)$

$$\begin{aligned}
 G_{\alpha}^2 &= \{A_g + T_g + 2T_u | A'\} + \{A_g + 2A_u + T_g | A''\} \\
 G_{\alpha}^{\#2} &= G_{\alpha}^{\#2} = \{A_g + T_g + 2T_u | A'\} + \{A_g + E_u + T_g | A''\}
 \end{aligned}$$

$\mathcal{R}_1(0), \mathcal{R}_1(T_d)$

$$E_{\frac{1}{2}}^2 = E_{\frac{2}{2}}^2 = \{T_1 | A'\} + \{A_1 | A''\}$$

$$G_{\frac{1}{2}}^2 = \{A_2 + 2T_1 + T_2 | A'\} + \{A_1 + E + T_2 | A''\}$$

$\mathcal{R}_2(0), \mathcal{R}_2(T_d)$

$$G_{\frac{2}{2}}^2 = \{A_1 + T_1 + 2T_2 | A'\} + \{A_1 + 2A_2 + T_1 | A''\}$$

$$G_{\frac{3}{2}}^2 = \{A_1 + T_1 + 2T_2 | A'\} + \{A_2 + E + T_1 | A''\}$$

$\mathcal{R}_1(0_h)$

$$G_{\alpha}^2 = \{A_{1u} + T_{1g} + T_{2g} + T_{2u} | A'\} + \{A_{1g} + A_{2g} + A_{2u} + T_{1u} | A''\}$$

$$K_{\alpha}^2 = \{A_{1g} + A_{2g} + 2A_{1u} + E_u + 3T_{1g} + T_{1u} + 3T_{2g} + 3T_{2u} | A'\} + \{A_{1g} + A_{2g} + 2A_{2u} + 2E_g + E_u + T_{1g} + 3T_{1u} + T_{2g} + T_{2u} | A''\}$$

$$E_{\beta}^2 = \{A_{1g} + A_{2g} + A_{2u} | A'\} + \{A_{1u} | A''\}$$

$$G_{\beta}^2 = \{A_{1g} + A_{2g} + 2A_{2u} + 2E_g + E_u | A'\} + \{A_{1g} + 2A_{1u} + A_{2g} + E_u | A''\}$$

$$I_{\beta}^2 = \{A_{1g} + A_{2g} + A_{2u} + 2E_g + E_u + T_{1g} + 2T_{1u} + T_{2g} | A'\} + \{A_{1u} + E_u + T_{1g} + T_{2g} + 2T_{2u} | A''\}$$

$$E_{\alpha\beta g}^{\prime 2} = E_{\alpha\beta g}^{\prime\prime 2} = E_{\alpha\beta u}^{\prime 2} = E_{\alpha\beta u}^{\prime\prime 2} = \{T_{1g} | A'\} + \{A_{1g} | A''\}$$

$$G_{\alpha\beta g}^2 = G_{\alpha\beta u}^2 = \{A_{2g} + 2T_{1g} + T_{2g} | A'\} + \{A_{1g} + E_g + T_{2g} | A''\}$$

$\mathcal{R}_2(0_h)$

$$G_{\alpha g}^{\prime 2} = G_{\alpha u}^{\prime 2} = \{A_{1g} + T_{1g} + 2T_{2g} | A'\} + \{A_{2g} + E_g + T_{1g} | A''\}$$

$$G_{\alpha g}^{\prime\prime 2} = G_{\alpha u}^{\prime\prime 2} = \{A_{1g} + T_{1g} + 2T_{2g} | A'\} + \{A_{1g} + 2A_{2g} + T_{1g} | A''\}$$

$$E_{1\beta}^2 = \{A_{1g} + A_{1u} + A_{2u} | A'\} + \{A_{2g} | A''\}$$

$$E_{2\beta}^2 = E_{3\beta}^2 = \{A_{1g} + E_u | A'\} + \{A_{2g} | A''\}$$

$$I_{\beta}^2 = \{A_{1g} + A_{1u} + A_{2u} + E_g + 2E_u + T_{1u} + 2T_{2g} + T_{2u} | A'\} + \{A_{2g} + E_g + 2T_{1g} + T_{1u} + T_{2u} | A''\}$$

$$G_{1\alpha\beta}^2 = \{A_{1g} + T_{1u} + T_{2g} + T_{2u} | A'\} + \{A_{1u} + A_{2g} + A_{2u} + T_{1g} | A''\}$$

$$G_{2\alpha\beta}^2 = G_{3\alpha\beta}^2 = \{A_{1g} + T_{1u} + T_{2g} + T_{2u} | A'\} + \{A_{2g} + E_u + T_{1g} | A''\}$$

$\mathcal{R}_3(0_h)$

$$G_{\alpha g}^{\prime 2} = G_{\alpha u}^{\prime 2} = \{A_{1g} + T_{1g} + 2T_{2g} | A'\} + \{A_{2g} + E_g + T_{1g} | A''\}$$

$$G_{\alpha g}^{\prime\prime 2} = G_{\alpha u}^{\prime\prime 2} = \{A_{1g} + T_{1g} + 2T_{2g} | A'\} + \{A_{1g} + 2A_{2g} + T_{1g} | A''\}$$

$$E_{1\beta}^2 = \{A_{1u} + A_{2g} + A_{2u} | A'\} + \{A_{1g} | A''\}$$

$$E_{2\beta}^2 = E_{3\beta}^2 = \{A_{2g} + E_u | A'\} + \{A_{1g} | A''\}$$

$$I_{\beta}^2 = \{A_{1u} + A_{2g} + A_{2u} + E_g + 2E_u + 2T_{1g} + T_{1u} + T_{2u} | A'\} + \{A_{1g} + E_g + T_{1u} + 2T_{2g} + T_{2u} | A''\}$$

$$G_{1\alpha\beta}^2 = \{A_{2g} + T_{1g} + T_{1u} + T_{2u} | A'\} + \{A_{1g} + A_{1u} + A_{2u} + T_{2g} | A''\}$$

$$G_{2\alpha\beta}^2 = G_{3\alpha\beta}^2 = \{A_{2g} + T_{1g} + T_{1u} + T_{2u} | A'\} + \{A_{1g} + E_u + T_{2g} | A''\}$$

$\mathcal{R}_4(O_h)$

$$G_\alpha^2 = \{A_{2g} + T_{1g} + T_{1u} + T_{2u} | A'\} + \{A_{1g} + A_{1u} + A_{2u} + T_{2g} | A''\}$$

$$K_\alpha^2 = \{A_{1g} + 2A_{1u} + A_{2g} + E_g + 2T_{1g} + 3T_{1u} + 2T_{2g} + 3T_{2u} | A'\} +$$

$$+ \{A_{1g} + A_{2g} + 2A_{2u} + E_g + 2E_u + 2T_{1g} + 2T_{1u} + 2T_{2g} | A''\}$$

$$E_\beta^2 = \{A_{1g} + A_{2g} + A_{2u} | A'\} + \{A_{1u} | A''\}$$

$$G_\beta^2 = \{A_{1g} + A_{2g} + 2A_{2u} + 2E_g + E_u | A'\} + \{A_{1g} + 2A_{1u} + A_{2g} + E_u | A''\}$$

$$I_\beta^2 = \{A_{1g} + A_{2g} + A_{2u} + 2E_g + E_u + T_{1g} + 2T_{1u} + T_{2g} | A'\} + \{A_{1u} + E_u + T_{1g} + T_{2g} + 2T_{2u} | A''\}$$

$$G_{1\alpha\beta}^2 = G_{2\alpha\beta}^2 = \{A_{1g} + T_{1g} + 2T_{2u} | A'\} + \{A_{1g} + 2A_{2u} + T_{1g} | A''\}$$

$$K_{\alpha\beta}^2 = \{A_{1g} + A_{1u} + 2A_{2g} + A_{2u} + 2E_g + 3T_{1g} + 3T_{1u} + T_{2g} + 3T_{2u} | A'\} +$$

$$+ \{2A_{1g} + A_{1u} + A_{2u} + E_g + 2E_u + T_{1g} + T_{1u} + 3T_{2g} + T_{2u} | A''\}$$

$\mathcal{R}(I)$

$$E_{1/2}^2 = \{T_1 | A'\} + \{A | A''\}$$

$$E_{7/2}^2 = \{T_2 | A'\} + \{A | A''\}$$

$$G_{3/2}^2 = \{T_1 + T_2 + G | A'\} + \{A + H | A''\}$$

$$I_{5/2}^2 = \{2T_1 + 2T_2 + G + H | A'\} + \{A + G + 2H | A''\}$$

$\mathcal{R}_1(I_h)$

$$E_{1/2g}^2 = E_{1/2u}^2 = \{T_{1g} | A'\} + \{A_g | A''\}$$

$$E_{7/2g}^2 = E_{7/2u}^2 = \{T_{2g} | A'\} + \{A_g | A''\}$$

$$G_{3/2g}^2 = G_{3/2u}^2 = \{T_{1g} + T_{2g} + G_g | A'\} + \{A_g + H_g | A''\}$$

$$I_{5/2g}^2 = I_{5/2u}^2 = \{2T_{1g} + 2T_{2g} + G_g + H_g | A'\} + \{A_g + G_g + 2H_g | A''\}$$

$\mathcal{R}_2(I_h)$

$$G_{1\alpha}^2 = \{A_g + T_{1g} + 2T_{1u} | A'\} + \{A_g + 2A_u + T_{1g} | A''\}$$

$$G_{2\alpha}^2 = \{A_g + T_{2g} + 2T_{2u} | A'\} + \{A_g + 2A_u + T_{2g} | A''\}$$

$$K_\alpha^2 = \{A_g + T_{1g} + 2T_{1u} + T_{2g} + 2T_{2u} + G_g + 2G_u + H_g | A'\} +$$

$$+ \{A_g + 2A_u + T_{1g} + T_{2g} + G_g + H_g + 2H_u | A''\}$$

$$I_\alpha^2 = \{A_g + 2T_{1g} + 4T_{1u} + 2T_{2g} + 4T_{2u} + 2G_g + 2G_u + 3H_g + 2H_u | A'\} +$$

$$+ \{A_g + 2A_u + 2T_{1g} + 2T_{2g} + 2G_g + 2G_u + 3H_g + 4H_u | A''\}$$

$\mathcal{R}_1(K_h)$

$$D_{(j+\frac{1}{2})g}^2 = D_{(j+\frac{1}{2})u}^2 = \left\{ \sum_{n=1}^{n=j+1} D_{(2n-1)g} | A'\right\} + \left\{ \sum_{n=1}^{n=j+1} D_{(2n-2)g} | A''\right\}$$

$\mathcal{R}_2(K_h)$

$$D_{(j+\frac{1}{2})\alpha}^2 = \left\{ \sum_{n=0}^{n=2j+1} D_{ng} + 2 \sum_{n=1}^{n=j+1} D_{(2n-1)u} | A'\right\} + \left\{ \sum_{n=0}^{n=2j+1} D_{ng} + 2 \sum_{n=1}^{n=j+1} D_{(2n-2)u} | A''\right\}$$

Table 4-21 The symmetrized squares of those representations of the representation groups which yield the projective representations of the point groups.

$\mathcal{R}_1(C_{4nh})$

$$\begin{aligned} E_{n\alpha}^3 &= \{2E_{n\alpha}|A_1\} + \{E_{n\alpha}|E\} \\ E_{2n\alpha}^3 &= \{2E_{2n\alpha}|A_1\} + \{E_{2n\alpha}|E\} \\ G_{\frac{n}{3}\alpha}^3 &= \{4E_{n\alpha} + 3G_{l\alpha}|A_1\} + \{G_{l\alpha}|A_2\} + \{2E_{n\alpha} + 4G_{l\alpha}|E\} \\ G_{\frac{2n}{3}\alpha}^3 \ (l \bmod 3 \neq 0) &= \{3G_{l\alpha} + 2G_{\{n-|n-3l \bmod 2n\}\alpha}|A_1\} + \{G_{l\alpha}|A_2\} + \\ &\quad + \{4G_{l\alpha} + G_{\{n-|n-3l \bmod 2n\}\alpha}|E\} \end{aligned}$$

$\mathcal{R}_2(C_{4nh})$

$$\begin{aligned} E_{\alpha}^3 &= \{2E_{\alpha}|A_1\} + \{E_{\alpha}|E\} \\ G_{\frac{2n}{3}\alpha}^3 &= \{4E_{\alpha} + 3G_{l\alpha}|A_1\} + \{G_{l\alpha}|A_2\} + \{2E_{\alpha} + 4G_{l\alpha}|E\} \\ G_{l\alpha}^3 \ (l \neq \frac{2n}{3}) &= \{3G_{l\alpha} + 2G_{\{n+\frac{1}{2}-|n-(3l-\frac{3}{2}) \bmod 2n\}\alpha}|A_1\} + \{G_{l\alpha}|A_2\} + \\ &\quad + \{4G_{l\alpha} + G_{\{n+\frac{1}{2}-|n-(3l-\frac{3}{2}) \bmod 2n\}\alpha}|E\} \end{aligned}$$

$\mathcal{R}_1(C_{(4n-2)h})$

$$\begin{aligned} E_{(2n-1)\alpha}^3 &= \{2E_{(2n-1)\alpha}|A_1\} + \{E_{(2n-1)\alpha}|E\} \\ G_{\frac{2n-1}{3}\alpha}^3 &= \{3G_{l\alpha} + 4E_{(2n-1)\alpha}|A_1\} + \{G_{l\alpha}|A_2\} + \{2E_{(2n-1)\alpha} + 4G_{l\alpha}|E\} \\ G_{l\alpha}^3 \ (l \neq (2n-1)/3) &= \{3G_{l\alpha} + 2G_{\{n-\frac{1}{2}-|n-\frac{1}{2}-3l \bmod (2n-1)\}\alpha}|A_1\} + \{G_{l\alpha}|A_2\} + \\ &\quad + \{4G_{l\alpha} + G_{\{n-\frac{1}{2}-|n-\frac{1}{2}-3l \bmod (2n-1)\}\alpha}|E\} \end{aligned}$$

$\mathcal{R}_2(C_{(4n-2)h})$

$$\begin{aligned} E_{\alpha}^3 &= \{2E_{\alpha}|A_1\} + \{E_{\alpha}|E\} \\ G_{\frac{2n-1}{3}\alpha}^3 &= \{4E_{\alpha} + 3G_{l\alpha}|A_1\} + \{G_{l\alpha}|A_2\} + \{2E_{\alpha} + 4G_{l\alpha}|E\} \\ G_{l\alpha}^3 \ (l \neq (2n-1)/3) &= \{3G_{l\alpha} + 2G_{\{2n-|n-\frac{1}{2}-(3l-\frac{3}{2}) \bmod (2n-1)\}\alpha}|A_1\} + \{G_{l\alpha}|A_2\} + \\ &\quad + \{4G_{l\alpha} + G_{\{2n-|n-\frac{1}{2}-(3l-\frac{3}{2}) \bmod (2n-1)\}\alpha}|E\} \end{aligned}$$

$\mathcal{R}_1(D_{2n}), \mathcal{R}_1(C_{2nv}), \mathcal{R}_1(D_{nd}), \mathcal{R}_1(D_{nh}) \ (n \text{ odd})$

$$E_{l\alpha}^3 = \{E_{l\alpha} + E_{\{2n-|2n-(6l-3) \bmod 4n\}\alpha}|A_1\} + \{E_{l\alpha}|E\}$$

$\mathcal{R}_2(D_{2n}), \mathcal{R}_2(C_{2nv}), \mathcal{R}_2(D_{nd}), \mathcal{R}_2(D_{nh}) \ (n \text{ odd})$

$$E_{l\alpha}^3 = \{E_{l\alpha} + E_{\{2n-|2n-(6l-3) \bmod 4n\}\alpha}|A_1\} + \{E_{l\alpha}|E\}$$

$\mathcal{R}_3(D_{4n}), \mathcal{R}_3(C_{4nv}), \mathcal{R}_3(D_{2nd})$

$$\begin{aligned} G_{l\alpha}^3 &= \{3G_{l\alpha} + 2G_{\frac{1}{2} + (3l-\frac{3}{2}) \bmod 2n}|A_1\} + \{G_{l\alpha}|A_2\} + \{4G_{l\alpha} + \\ &\quad + G_{\frac{1}{2} + (3l-\frac{3}{2}) \bmod 2n}|E\} \end{aligned}$$

$$\mathcal{R}_3(D_{4n-2}), \mathcal{R}_3(C_{4nv}), \mathcal{R}_3(D_{(2n-1)d}), \mathcal{R}_3(D_{(2n-1)h})$$

$$E_\alpha^3 = \{2E_\alpha | A_1\} + \{E_\alpha | \mathcal{E}\}$$

$$G_{\frac{2n-1}{3}\alpha}^3 = \{4E_\alpha + 3G_{\frac{2n-1}{3}\alpha} | A_1\} + \{G_{\frac{2n-1}{3}\alpha} | A_2\} + \{2E_\alpha + 4G_{\frac{2n-1}{3}\alpha} | \mathcal{E}\}$$

$$G_{l\alpha}^3 (l \neq (2n-1)/3) = \{3G_{l\alpha} + 2G_{\{(n-\frac{1}{2}-|n-\frac{1}{2}-3l)\} \bmod n}\alpha} | A_1\} + \{G_{l\alpha} | A_2\} + \{4G_{l\alpha} + G_{\{(n-\frac{1}{2}-|n-\frac{1}{2}-3l)\} \bmod n}\alpha} | \mathcal{E}\}$$

$$\mathcal{Q}_1(D_{4nh})$$

$$E_{l\alpha}^3 = \{E_{l\alpha} + E_{\{4n+\frac{1}{2}-|4n-(3l-\frac{3}{2})\} \bmod 4n}\alpha} | A_1\} + \{E_{l\alpha} | \mathcal{E}\}$$

$$E_{1\beta}^3 = \{2E_{1\beta} | A_1\} + \{E_{1\beta} | \mathcal{E}\}$$

$$E_{2\beta}^3 = \{2E_{2\beta} | A_1\} + \{E_{2\beta} | \mathcal{E}\}$$

$$G_{\frac{2n}{3}\beta}^3 = \{4E_{2\beta} + 3G_{\frac{2n}{3}\beta} | A_1\} + \{G_{\frac{2n}{3}\beta} | A_2\} + \{2E_{2\beta} + 4G_{\frac{2n}{3}\beta} | \mathcal{E}\}$$

$$G_{\frac{4n}{3}\beta}^3 = \{4E_{1\beta} + 3G_{\frac{4n}{3}\beta} | A_1\} + \{G_{\frac{4n}{3}\beta} | A_2\} + \{2E_{1\beta} + 4G_{\frac{4n}{3}\beta} | \mathcal{E}\}$$

$$G_{l\beta}^3 (l \bmod \frac{2n}{3} \neq 0) = \{3G_{l\beta} + 2G_{\{4n-|4n-3l \bmod 2n\}\beta} | A_1\} + \{G_{l\beta} | A_2\} + \{4G_{l\beta} + G_{\{4n-|4n-3l \bmod 2n\}\beta} | \mathcal{E}\}$$

$$E_{1\gamma}^3 = \{2E_{1\gamma} | A_1\} + \{E_{1\gamma} | \mathcal{E}\}$$

$$E_{2\gamma}^3 = \{2E_{2\gamma} | A_1\} + \{E_{2\gamma} | \mathcal{E}\}$$

$$G_\gamma^3 = \{5G_\gamma | A_1\} + \{G_\gamma | A_2\} + \{5G_\gamma | \mathcal{E}\}$$

$$G_{\frac{n}{3}\gamma}^3 = \{3G_{\frac{n}{3}\gamma} + 2G_\gamma | A_1\} + \{G_{\frac{n}{3}\gamma} | A_2\} + \{4G_{\frac{n}{3}\gamma} + G_\gamma | \mathcal{E}\}$$

$$G_{\frac{2n}{3}\gamma}^3 = \{2E_{1\gamma} + 2E_{2\gamma} + 3G_{\frac{2n}{3}\gamma} | A_1\} + \{G_{\frac{2n}{3}\gamma} | A_2\} + \{E_{1\gamma} + E_{2\gamma} + 4G_{\frac{2n}{3}\gamma} | \mathcal{E}\}$$

$$G_{l\gamma}^3 (l \bmod \frac{2n}{3} \neq 0) = \{3G_{l\gamma} + 2G_{\{(\frac{1}{2}n + |\frac{1}{2}n - 3l\}) \bmod n\}\gamma} | A_1\} + \{G_{l\gamma} | A_2\} + \{4G_{l\gamma} + G_{\{(\frac{1}{2}n + |\frac{1}{2}n - 3l\}) \bmod n\}\gamma} | \mathcal{E}\}$$

$$G_{l\alpha\beta}^3 = \{3G_{l\alpha\beta} + 2G_{\{2n+\frac{1}{2}-|2n-(3l-\frac{3}{2})\} \bmod 4n\}\alpha\beta} | A_1\} + \{G_{l\alpha\beta} | A_2\} + \{4G_{l\alpha\beta} + G_{\{2n+\frac{1}{2}-|2n-(3l-\frac{3}{2})\} \bmod 4n\}\alpha\beta} | \mathcal{E}\}$$

$$G_{l\alpha\gamma}^3 = \{3G_{l\alpha\gamma} + 2G_{\{n+\frac{1}{2}-|n-(3l-\frac{3}{2})\} \bmod 4n\}\alpha\gamma} | A_1\} + \{G_{l\alpha\gamma} | A_2\} + \{4G_{l\alpha\gamma} + G_{\{n+\frac{1}{2}-|n-(3l-\frac{3}{2})\} \bmod 4n\}\alpha\gamma} | \mathcal{E}\}$$

$$E_{1\gamma\beta}^3 = \{2E_{1\gamma\beta} | A_1\} + \{E_{1\gamma\beta} | \mathcal{E}\}$$

$$E_{2\gamma\beta}^3 = \{2E_{2\gamma\beta} | A_1\} + \{E_{2\gamma\beta} | \mathcal{E}\}$$

$$G_{\gamma\beta}^3 = \{5G_{\gamma\beta} | A_1\} + \{G_{\gamma\beta} | A_2\} + \{5G_{\gamma\beta} | \mathcal{E}\}$$

$$G_{\frac{n}{3}\gamma\beta}^3 = \{3G_{\frac{n}{3}\gamma\beta} + 2G_{\gamma\beta} | A_1\} + \{G_{\frac{n}{3}\gamma\beta} | A_2\} + \{4G_{\frac{n}{3}\gamma\beta} + G_{\gamma\beta} | \mathcal{E}\}$$

$$G_{\frac{2n}{3}\gamma\beta}^3 = \{2E_{1\gamma\beta} + 2E_{2\gamma\beta} + 3G_{\frac{2n}{3}\gamma\beta} | A_1\} + \{G_{\frac{2n}{3}\gamma\beta} | A_2\} + \{E_{1\gamma\beta} + E_{2\gamma\beta} + 4G_{\frac{2n}{3}\gamma\beta} | \mathcal{E}\}$$

$$G_{l\gamma\beta}^3 (l \bmod \frac{n}{3} \neq 0) = \{3G_{l\gamma\beta} + 2G_{\{(\frac{1}{2}n + |\frac{1}{2}n - 3l\}) \bmod n\}\gamma\beta} | A_1\} + \{G_{l\gamma\beta} | A_2\} + \{4G_{l\gamma\beta} + G_{\{(\frac{1}{2}n + |\frac{1}{2}n - 3l\}) \bmod n\}\gamma\beta} | \mathcal{E}\}$$

$$G_{l\alpha\gamma\beta}^3 = \{3G_{l\alpha\gamma\beta} + 2G_{\{(n+\frac{1}{2}-|n-(3l-\frac{3}{2})\}) \bmod n\}\alpha\gamma\beta} | A_1\} + \{G_{l\alpha\gamma\beta} | A_2\} + \{4G_{l\alpha\gamma\beta} + G_{\{(n+\frac{1}{2}-|n-(3l-\frac{3}{2})\}) \bmod n\}\alpha\gamma\beta} | \mathcal{E}\}$$

$\mathcal{D}_2(D_{4n})$

$$G_{\lambda\alpha}^3 = \{3G_{\lambda\alpha} + 2G_{\lfloor \frac{1}{2} + (3l - \frac{3}{2}) \bmod 2n \rfloor \alpha} | A_1 \} + \{G_{\lambda\alpha} | A_2 \} + \{4G_{\lambda\alpha} + G_{\lfloor \frac{1}{2} + (3l - \frac{3}{2}) \bmod 2n \rfloor \alpha} | \mathcal{E} \}$$

$$E_{1\beta}^3 = \{2E_{1\beta} | A_1 \} + \{E_{1\beta} | \mathcal{E} \}$$

$$E_{2\beta}^3 = \{2E_{2\beta} | A_1 \} + \{E_{2\beta} | \mathcal{E} \}$$

$$G_{\lambda\beta}^3 = \{5G_{\lambda\beta} | A_1 \} + \{G_{\lambda\beta} | A_2 \} + \{5G_{\lambda\beta} | \mathcal{E} \}$$

$$E_{1\gamma}^3 = \{2E_{1\gamma} | A_1 \} + \{E_{1\gamma} | \mathcal{E} \}$$

$$E_{2\gamma}^3 = \{2E_{2\gamma} | A_1 \} + \{E_{2\gamma} | \mathcal{E} \}$$

$$G_{\gamma}^3 = \{5G_{\gamma} | A_1 \} + \{G_{\gamma} | A_2 \} + \{5G_{\gamma} | \mathcal{E} \}$$

$$G_{\lambda\gamma}^3 = \{3G_{\lambda\gamma} + 2G_{\lfloor n - |n - (6l - 3) \bmod 2n \rfloor \gamma} | A_1 \} + \{G_{\lambda\gamma} | A_2 \} + \{4G_{\lambda\gamma} + G_{\lfloor n - |n - (6l - 3) \bmod 2n \rfloor \gamma} | \mathcal{E} \}$$

$$G_{\lambda\alpha\beta}^3 = \{3G_{\lambda\alpha\beta} + 2G_{\lfloor 2n + \frac{1}{2} - |2n - (3l - \frac{3}{2}) \bmod 2n \rfloor \alpha\beta} | A_1 \} + \{G_{\lambda\alpha\beta} | A_2 \} + \{4G_{\lambda\alpha\beta} + G_{\lfloor 2n + \frac{1}{2} - |2n - (3l - \frac{3}{2}) \bmod 2n \rfloor \alpha\beta} | \mathcal{E} \}$$

$$G_{\lambda\alpha\gamma}^3 = \{3G_{\lambda\alpha\gamma} + 2G_{\lfloor n + \frac{1}{2} - |n - (3l - \frac{3}{2}) \bmod 2n \rfloor \alpha\gamma} | A_1 \} + \{G_{\lambda\alpha\gamma} | A_2 \} + \{4G_{\lambda\alpha\gamma} + G_{\lfloor n + \frac{1}{2} - |n - (3l - \frac{3}{2}) \bmod 2n \rfloor \alpha\gamma} | \mathcal{E} \}$$

$$G_{\beta\gamma}^3 = \{5G_{\beta\gamma} | A_1 \} + \{G_{\beta\gamma} | A_2 \} + \{5G_{\beta\gamma} | \mathcal{E} \}$$

$$E_{1\beta\gamma}^3 = \{2E_{1\beta\gamma} | A_1 \} + \{E_{1\beta\gamma} | \mathcal{E} \}$$

$$E_{2\beta\gamma}^3 = \{2E_{2\beta\gamma} | A_1 \} + \{E_{2\beta\gamma} | \mathcal{E} \}$$

$$G_{\lambda\beta\gamma}^3 = \{3G_{\lambda\beta\gamma} + 2G_{\lfloor \frac{1}{2}n + \frac{1}{2} - | \frac{1}{2}n - (3l - \frac{3}{2}) \bmod n \rfloor \beta\gamma} | A_1 \} + \{G_{\lambda\beta\gamma} | A_2 \} + \{4G_{\lambda\beta\gamma} + G_{\lfloor \frac{1}{2}n + \frac{1}{2} - | \frac{1}{2}n - (3l - \frac{3}{2}) \bmod n \rfloor \beta\gamma} | \mathcal{E} \}$$

$$G_{\lambda\alpha\beta\gamma}^3 = \{3G_{\lambda\alpha\beta\gamma} + 2G_{\lfloor n + \frac{1}{2} - |n - (3l - \frac{3}{2}) \bmod n \rfloor \alpha\beta\gamma} | A_1 \} + \{G_{\lambda\alpha\beta\gamma} | A_2 \} + \{4G_{\lambda\alpha\beta\gamma} + G_{\lfloor n + \frac{1}{2} - |n - (3l - \frac{3}{2}) \bmod n \rfloor \alpha\beta\gamma} | \mathcal{E} \}$$

$\mathcal{D}_1(D_{(4n-2)h})$

$$E_{\lambda\alpha}^3 = \{E_{\lambda\alpha} + E_{\lfloor 2n - \frac{1}{2} - |4n - 2 - (3l - \frac{3}{2}) \bmod (2n - 1) \rfloor \alpha} | A_1 \} + \{E_{\lambda\alpha} | \mathcal{E} \}$$

$$E_{1\beta}^3 = \{2E_{1\beta} | A_1 \} + \{E_{1\beta} | \mathcal{E} \}$$

$$E_{2\beta}^3 = \{2E_{2\beta} | A_1 \} + \{E_{2\beta} | \mathcal{E} \}$$

$$G_{\frac{2n-1}{3}\beta}^3 = \{4E_{2\beta} + 3G_{\frac{2n-1}{3}\beta} | A_1 \} + \{G_{\frac{2n-1}{3}\beta} | A_2 \} + \{2E_{2\beta} + 4G_{\frac{2n-1}{3}\beta} | \mathcal{E} \}$$

$$G_{\frac{4n-2}{3}\beta}^3 = \{4E_{1\beta} + 3G_{\frac{4n-2}{3}\beta} | A_1 \} + \{G_{\frac{4n-2}{3}\beta} | A_2 \} + \{2E_{1\beta} + 4G_{\frac{4n-2}{3}\beta} | \mathcal{E} \}$$

$$G_{\lambda\beta}^3 \ (l \bmod \frac{2n-1}{3} \neq 0) = \{3G_{\lambda\beta} + 2G_{\lfloor 4n - 2 - |4n - 2 - (3l) \bmod (4n - 2) \rfloor \beta} | A_1 \} + \{G_{\lambda\beta} | A_2 \} + \{4G_{\lambda\beta} + G_{\lfloor 4n - 2 - |4n - 2 - (3l) \bmod (4n - 2) \rfloor \beta} | \mathcal{E} \}$$

$$E_{1\gamma}^2 = \{2E_{1\gamma} | A_1 \} + \{E_{1\gamma} | \mathcal{E} \}$$

$$E_{2\gamma}^2 = \{2E_{2\gamma} | A_1 \} + \{E_{2\gamma} | \mathcal{E} \}$$

$$G_{\frac{2n-1}{3}\gamma}^3 = \{2E_{1\gamma} + 2E_{2\gamma} + 3G_{\frac{2n-1}{3}\gamma} | A_1 \} + \{G_{\frac{2n-1}{3}\gamma} | A_2 \} + \{E_{1\gamma} + E_{2\gamma} + 4G_{\frac{2n-1}{3}\gamma} | \mathcal{E} \}$$

$$G_{\lambda\delta}^3 (\lambda \neq (2n-1)/3) = \{3G_{\lambda\delta} + 2G_{\{(\frac{1}{2}n + \frac{1}{2}n - 3\ell)\bmod n\}\delta} | A_1\} + \{G_{\lambda\delta} | A_2\} + \{4G_{\lambda\delta} + G_{\{(\frac{1}{2}n + \frac{1}{2}n - 3\ell)\bmod n\}\delta} | \mathcal{E}\}$$

$$G_{\alpha\delta}^3 = \{5G_{\alpha\delta} | A_1\} + \{G_{\alpha\delta} | A_2\} + \{5G_{\alpha\delta} | \mathcal{E}\}$$

$$G_{\frac{2n-1}{3}\alpha\delta}^3 = \{2G_{\alpha\delta} + 3G_{\frac{2n-1}{3}\alpha\delta} | A_1\} + \{G_{\frac{2n-1}{3}\alpha\delta} | A_2\} + \{G_{\alpha\delta} + 4G_{\frac{2n-1}{3}\alpha\delta} | \mathcal{E}\}$$

$$G_{\lambda\alpha\delta}^3 (\lambda \neq (2n-1)/3) = \{3G_{\lambda\alpha\delta} + 2G_{\{n - |n - \frac{1}{2} - (3\ell - \frac{3}{2})\bmod(2n-1)\}\alpha\delta} | A_1\} + \{G_{\lambda\alpha\delta} | A_2\} + \{4G_{\lambda\alpha\delta} + G_{\{n - |n - \frac{1}{2} - (3\ell - \frac{3}{2})\bmod(2n-1)\}\alpha\delta} | \mathcal{E}\}$$

$$G_{\delta\beta}^3 = \{5G_{\delta\beta} | A_1\} + \{G_{\delta\beta} | A_2\} + \{5G_{\delta\beta} | \mathcal{E}\}$$

$$G_{\lambda\delta\beta}^3 = \{3G_{\lambda\delta\beta} + 2G_{\{(\frac{1}{2}n + \frac{1}{2}n - 3\ell)\bmod n\}\delta\beta} | A_1\} + \{G_{\lambda\delta\beta} | A_2\} + \{4G_{\lambda\delta\beta} + G_{\{(\frac{1}{2}n + \frac{1}{2}n - 3\ell)\bmod n\}\delta\beta} | \mathcal{E}\}$$

$$E_{1\alpha\beta\delta}^3 = \{2E_{1\alpha\beta\delta} | A_1\} + \{E_{1\alpha\beta\delta} | \mathcal{E}\}$$

$$E_{2\alpha\beta\delta}^3 = \{2E_{2\alpha\beta\delta} | A_1\} + \{E_{2\alpha\beta\delta} | \mathcal{E}\}$$

$$G_{\frac{2n-1}{3}\alpha\beta\delta}^3 = \{2E_{1\alpha\beta\delta} + 2E_{2\alpha\beta\delta} + 3G_{\frac{2n-1}{3}\alpha\beta\delta} | A_1\} + \{G_{\frac{2n-1}{3}\alpha\beta\delta} | A_2\} + \{E_{1\alpha\beta\delta} + E_{2\alpha\beta\delta} + 4G_{\frac{2n-1}{3}\alpha\beta\delta} | \mathcal{E}\}$$

$$G_{\lambda\alpha\beta\delta}^3 (\lambda \neq (2n-1)/3) = \{3G_{\lambda\alpha\beta\delta} + 2G_{\{(n - |n - \frac{1}{2} - (3\ell - \frac{3}{2})\bmod(2n-1)\}\alpha\beta\delta} | A_1\} + \{G_{\lambda\alpha\beta\delta} | A_2\} + \{4G_{\lambda\alpha\beta\delta} + G_{\{(n - |n - \frac{1}{2} - (3\ell - \frac{3}{2})\bmod(2n-1)\}\alpha\beta\delta} | \mathcal{E}\}$$

$\mathcal{R}_2(D_{(4n-2)h})$

$$E_{1\alpha}^3 = \{2E_{1\alpha} | A_1\} + \{E_{1\alpha} | \mathcal{E}\}$$

$$E_{2\alpha}^3 = \{2E_{2\alpha} | A_1\} + \{E_{2\alpha} | \mathcal{E}\}$$

$$G_{\frac{n-1}{3}\alpha}^3 = \{2E_{1\alpha} + 2E_{2\alpha} + 3G_{\frac{n-1}{3}\alpha} | A_1\} + \{G_{\frac{n-1}{3}\alpha} | A_2\} + \{E_{1\alpha} + E_{2\alpha} + 4G_{\frac{n-1}{3}\alpha} | \mathcal{E}\}$$

$$G_{\lambda\alpha}^3 (\lambda \neq \frac{1}{3}(n-1)) = \{3G_{\lambda\alpha} + 2G_{\{(n - |n - \frac{1}{2} - (3\ell - \frac{3}{2})\bmod n\}\alpha} | A_1\} + \{G_{\lambda\alpha} | A_2\} + \{4G_{\lambda\alpha} + G_{\{(n - |n - \frac{1}{2} - (3\ell - \frac{3}{2})\bmod n\}\alpha} | \mathcal{E}\}$$

$$E_{1\beta}^3 = \{2E_{1\beta} | A_1\} + \{E_{1\beta} | \mathcal{E}\}$$

$$E_{2\beta}^3 = \{2E_{2\beta} | A_1\} + \{E_{2\beta} | \mathcal{E}\}$$

$$G_{\frac{2n-1}{3}\beta}^3 = \{2E_{1\beta} + 2E_{2\beta} + 3G_{\frac{2n-1}{3}\beta} | A_1\} + \{G_{\frac{2n-1}{3}\beta} | A_2\} + \{E_{1\beta} + E_{2\beta} + 4G_{\frac{2n-1}{3}\beta} | \mathcal{E}\}$$

$$G_{\lambda\beta}^3 (\lambda \neq (2n-1)/3) = \{3G_{\lambda\beta} + 2G_{\{\frac{1}{2}n - \frac{1}{2}n - 3\ell\}\beta} | A_1\} + \{G_{\lambda\beta} | A_2\} + \{4G_{\lambda\beta} + G_{\{\frac{1}{2}n - \frac{1}{2}n - 3\ell\}\beta} | \mathcal{E}\}$$

$$E_{1\gamma}^3 = \{2E_{1\gamma} | A_1\} + \{E_{1\gamma} | \mathcal{E}\}$$

$$E_{2\gamma}^3 = \{2E_{2\gamma} | A_1\} + \{E_{2\gamma} | \mathcal{E}\}$$

$$G_{\frac{2n-1}{3}\gamma}^3 = \{4E_{2\gamma} + 3G_{\frac{2n-1}{3}\gamma} | A_1\} + \{G_{\frac{2n-1}{3}\gamma} | A_2\} + \{2E_{2\gamma} + 4G_{\frac{2n-1}{3}\gamma} | \mathcal{E}\}$$

$$G_{\frac{4n-2}{3}\gamma}^3 = \{4E_{1\gamma} + 3G_{\frac{4n-2}{3}\gamma} | A_1\} + \{G_{\frac{4n-2}{3}\gamma} | A_2\} + \{2E_{1\gamma} + 4G_{\frac{4n-2}{3}\gamma} | \mathcal{E}\}$$

$$\begin{aligned}
 G_{\ell\gamma}^3 (\ell \bmod \frac{2n-1}{3} \neq 0) &= \{3G_{\ell\gamma} + 2G_{\{(2n-1-|2n-3\ell-1|) \bmod (2n-1)\}\gamma} | A_1 \} + \\
 &\quad + \{G_{\ell\gamma} | A_2 \} + \{4G_{\ell\gamma} + G_{\{(2n-1-|2n-3\ell-1|) \bmod (2n-1)\}\gamma} | \mathcal{E} \} \\
 G_{\ell\alpha\beta}^3 &= \{3G_{\ell\alpha\beta} + 2G_{\{2n+\frac{3}{2}-|2n-1-(3\ell-\frac{3}{2}) \bmod (2n-1)\}\alpha\beta} | A_1 \} + \{G_{\ell\alpha\beta} | A_2 \} + \\
 &\quad + \{4G_{\ell\alpha\beta} + G_{\{2n+\frac{3}{2}-|2n-1-(3\ell-\frac{3}{2}) \bmod (2n-1)\}\alpha\beta} | \mathcal{E} \} \\
 E_{\alpha\delta}^3 &= \{5E_{\alpha\delta} | A_1 \} + \{E_{\alpha\delta} | A_2 \} + \{5E_{\alpha\delta} | \mathcal{E} \} \\
 G_{\frac{n+1}{3}\alpha\delta}^3 &= \{4E_{\alpha\delta} + 3G_{\frac{n+1}{3}\alpha\delta} | A_1 \} + \{G_{\frac{n+1}{3}\alpha\delta} | A_2 \} + \{2E_{\alpha\delta} + 4G_{\frac{n+1}{3}\alpha\delta} | \mathcal{E} \} \\
 G_{\ell\alpha\delta}^3 (\ell \neq (n+1)/3) &= \{3G_{\ell\alpha\delta} + 2G_{\{(n-|n-\frac{1}{2}-(3\ell-\frac{3}{2})|) \bmod n\}\alpha\delta} | A_1 \} + \{G_{\ell\alpha\delta} | A_2 \} + \\
 &\quad + \{4G_{\ell\alpha\delta} + G_{\{(n-|n-\frac{1}{2}-(3\ell-\frac{3}{2})|) \bmod n\}\alpha\delta} | \mathcal{E} \} \\
 E_{\delta\beta}^3 &= \{5E_{\delta\beta} | A_1 \} + \{E_{\delta\beta} | A_2 \} + \{5E_{\delta\beta} | \mathcal{E} \} \\
 G_{\frac{2n-1}{3}\delta\beta}^3 &= \{4E_{\delta\beta} + 3G_{\frac{2n-1}{3}\delta\beta} | A_1 \} + \{G_{\frac{2n-1}{3}\delta\beta} | A_2 \} + \{2E_{\delta\beta} + 4G_{\frac{2n-1}{3}\delta\beta} | \mathcal{E} \} \\
 G_{\ell\delta\beta}^3 (\ell \neq (2n-1)/3) &= \{3G_{\ell\delta\beta} + 2G_{\{(2n-1-|2n-3\ell-1|) \bmod (2n-1)\}\delta\beta} | A_1 \} + \\
 &\quad + \{G_{\ell\delta\beta} | A_2 \} + \{4G_{\ell\delta\beta} + G_{\{(2n-1-|2n-3\ell-1|) \bmod (2n-1)\}\delta\beta} | \mathcal{E} \} \\
 E_{\ell\alpha\beta\delta}^3 &= \{E_{\ell\alpha\beta\delta} + E_{\{4n-\frac{3}{2}-|4n-2-(3\ell-\frac{3}{2}) \bmod (4n-2)\}\alpha\beta\delta} | A_1 \} + \{E_{\ell\alpha\beta\delta} | \mathcal{E} \}
 \end{aligned}$$

$\mathcal{R}(T)$

$$\begin{aligned}
 E_{\frac{1}{2}}^3 &= \{G_{\frac{3}{2}} | A_1 \} + \{E_{\frac{1}{2}} | \mathcal{E} \} \\
 G_{\frac{3}{2}}^3 &= \{2E_{\frac{1}{2}} + 4G_{\frac{3}{2}} | A_1 \} + \{G_{\frac{3}{2}} | A_2 \} + \{4E_{\frac{1}{2}} + 3G_{\frac{3}{2}} | \mathcal{E} \}
 \end{aligned}$$

$\mathcal{R}_1(T_u)$

$$\begin{aligned}
 E_{\frac{1}{2}g}^3 &= \{G_{\frac{3}{2}g} | A_1 \} + \{E_{\frac{1}{2}g} | \mathcal{E} \} \\
 E_{\frac{1}{2}u}^3 &= \{G_{\frac{3}{2}u} | A_1 \} + \{E_{\frac{1}{2}u} | \mathcal{E} \} \\
 G_{\frac{3}{2}g}^3 &= \{2E_{\frac{1}{2}g} + 4G_{\frac{3}{2}g} | A_1 \} + \{G_{\frac{3}{2}g} | A_2 \} + \{4E_{\frac{1}{2}g} + 3G_{\frac{3}{2}g} | \mathcal{E} \} \\
 G_{\frac{3}{2}u}^3 &= \{2E_{\frac{1}{2}u} + 4G_{\frac{3}{2}u} | A_1 \} + \{G_{\frac{3}{2}u} | A_2 \} + \{4E_{\frac{1}{2}u} + 3G_{\frac{3}{2}u} | \mathcal{E} \}
 \end{aligned}$$

$\mathcal{R}_2(T_u)$

$$\begin{aligned}
 G_{\alpha}^3 &= \{G_{\alpha} + 2G'_{\alpha} + 2G''_{\alpha} | A_1 \} + \{G_{\alpha} | A_2 \} + \{3G_{\alpha} + G'_{\alpha} + G''_{\alpha} | \mathcal{E} \} \\
 G_{\alpha}'^3 &= \{G_{\alpha} + 2G'_{\alpha} + 2G''_{\alpha} | A_1 \} + \{G'_{\alpha} | A_2 \} + \{2G_{\alpha} + 2G'_{\alpha} + G''_{\alpha} | \mathcal{E} \} \\
 G_{\alpha}''^3 &= \{G_{\alpha} + 2G'_{\alpha} + 2G''_{\alpha} | A_1 \} + \{G''_{\alpha} | A_2 \} + \{2G_{\alpha} + 2G'_{\alpha} + G''_{\alpha} | \mathcal{E} \}
 \end{aligned}$$

$\mathcal{R}_1(0), \mathcal{R}_1(T_d)$

$$\begin{aligned}
 E_{\frac{1}{2}}^3 &= \{G_{\frac{3}{2}} | A_1 \} + \{E_{\frac{1}{2}} | \mathcal{E} \} \\
 E_{\frac{5}{2}}^3 &= \{G_{\frac{3}{2}} | A_1 \} + \{E_{\frac{5}{2}} | \mathcal{E} \} \\
 G_{\frac{3}{2}}^3 &= \{E_{\frac{1}{2}} + E_{\frac{5}{2}} + 2G_{\frac{3}{2}} | A_1 \} + \{G_{\frac{3}{2}} | A_2 \} + \{2E_{\frac{1}{2}} + 2E_{\frac{5}{2}} + 3G_{\frac{3}{2}} | \mathcal{E} \}
 \end{aligned}$$

$\mathcal{R}_2(0), \mathcal{R}_2(T_d)$

$$\begin{aligned}
 G_{\frac{1}{2}}^3 &= \{G_{\frac{1}{2}} + 4G_{\frac{3}{2}} | A_1 \} + \{G_{\frac{1}{2}} | A_2 \} + \{3G_{\frac{1}{2}} + 2G_{\frac{3}{2}} | \mathcal{E} \} \\
 G_{\frac{3}{2}}^3 &= \{G_{\frac{1}{2}} + 4G_{\frac{3}{2}} | A_1 \} + \{G_{\frac{3}{2}} | A_2 \} + \{2G_{\frac{1}{2}} + 3G_{\frac{3}{2}} | \mathcal{E} \}
 \end{aligned}$$

$\mathcal{R}_1(O_h)$

$$\begin{aligned}
 G_\alpha^3 &= \{G_\alpha + 2K_\alpha | A_1\} + \{G_\alpha | A_2\} + \{3G_\alpha + K_\alpha | E\} \\
 K_\alpha^3 &= \{8G_\alpha + 11K_\alpha | A_1\} + \{4G_\alpha + 5K_\alpha | A_2\} + \{14G_\alpha + 14K_\alpha | E\} \\
 E_\beta^3 &= \{2E_\beta | A_1\} + \{E_\beta | E\} \\
 G_\beta^3 &= \{4E_\beta + 3G_\beta | A_1\} + \{G_\beta | A_2\} + \{2E_\beta + 4G_\beta | E\} \\
 I_\beta^3 &= \{2E_\beta + G_\beta + 8I_\beta | A_1\} + \{2E_\beta + G_\beta + 2I_\beta | A_2\} + \{2E_\beta + 3G_\beta + 9I_\beta | E\} \\
 E_{\alpha\beta\gamma}^{\prime 3} &= \{G_{\alpha\beta\gamma} | A_1\} + \{E'_{\alpha\beta\gamma} | E\} \\
 E_{\alpha\beta\gamma}^{\prime\prime 3} &= \{G_{\alpha\beta\gamma} | A_1\} + \{E''_{\alpha\beta\gamma} | E\} \\
 E_{\alpha\beta\mu}^{\prime 3} &= \{G_{\alpha\beta\mu} | A_1\} + \{E'_{\alpha\beta\mu} | E\} \\
 E_{\alpha\beta\mu}^{\prime\prime 3} &= \{G_{\alpha\beta\mu} | A_1\} + \{E''_{\alpha\beta\mu} | E\} \\
 G_{\alpha\beta\gamma}^3 &= \{E'_{\alpha\beta\gamma} + E''_{\alpha\beta\gamma} + 4G_{\alpha\beta\gamma} | A_1\} + \{G_{\alpha\beta\gamma} | A_2\} + \{2E'_{\alpha\beta\gamma} + 2E''_{\alpha\beta\gamma} + 3G_{\alpha\beta\gamma} | E\} \\
 G_{\alpha\beta\mu}^3 &= \{E'_{\alpha\beta\mu} + E''_{\alpha\beta\mu} + 4G_{\alpha\beta\mu} | A_1\} + \{G_{\alpha\beta\mu} | A_2\} + \{2E'_{\alpha\beta\mu} + 2E''_{\alpha\beta\mu} + 3G_{\alpha\beta\mu} | E\}
 \end{aligned}$$

$\mathcal{R}_2(O_h)$

$$\begin{aligned}
 G'_{\alpha\gamma} &= \{4G'_{\alpha\gamma} + G''_{\alpha\gamma} | A_1\} + \{G'_{\alpha\gamma} | A_2\} + \{3G'_{\alpha\gamma} + 2G''_{\alpha\gamma} | E\} \\
 G''_{\alpha\gamma} &= \{4G'_{\alpha\gamma} + G''_{\alpha\gamma} | A_1\} + \{G''_{\alpha\gamma} | A_2\} + \{2G'_{\alpha\gamma} + 3G''_{\alpha\gamma} | E\} \\
 G'_{\alpha u} &= \{4G'_{\alpha u} + G''_{\alpha u} | A_1\} + \{G'_{\alpha u} | A_2\} + \{3G'_{\alpha u} + 2G''_{\alpha u} | E\} \\
 G''_{\alpha u} &= \{4G'_{\alpha u} + G''_{\alpha u} | A_1\} + \{G''_{\alpha u} | A_2\} + \{2G'_{\alpha u} + 3G''_{\alpha u} | E\} \\
 E_{1\beta}^3 &= \{2E_{1\beta} | A_1\} + \{E_{1\beta} | E\} \\
 E_{2\beta}^3 &= \{2E_{1\beta} | A_1\} + \{E_{2\beta} | E\} \\
 E_{3\beta}^3 &= \{2E_{1\beta} | A_1\} + \{E_{3\beta} | E\} \\
 I_\beta^3 &= \{2E_{1\beta} + E_{2\beta} + E_{3\beta} + 8I_\beta | A_1\} + \{2E_{1\beta} + E_{2\beta} + E_{3\beta} | A_2\} + \\
 &\quad + \{2E_{1\beta} + 3E_{2\beta} + 3E_{3\beta} + 9I_\beta | E\} \\
 G_{1\alpha\beta}^3 &= \{G_{1\alpha\beta} + 2G_{2\alpha\beta} + 2G_{3\alpha\beta} | A_1\} + \{G_{1\alpha\beta} | A_2\} + \{3G_{1\alpha\beta} + G_{2\alpha\beta} + G_{3\alpha\beta} | E\} \\
 G_{2\alpha\beta}^3 &= \{G_{1\alpha\beta} + 2G_{2\alpha\beta} + 2G_{3\alpha\beta} | A_1\} + \{G_{2\alpha\beta} | A_2\} + \{2G_{1\alpha\beta} + 2G_{2\alpha\beta} + G_{3\alpha\beta} | E\} \\
 G_{3\alpha\beta}^3 &= \{G_{1\alpha\beta} + 2G_{2\alpha\beta} + 2G_{3\alpha\beta} | A_1\} + \{G_{3\alpha\beta} | A_2\} + \{2G_{1\alpha\beta} + G_{2\alpha\beta} + 2G_{3\alpha\beta} | E\}
 \end{aligned}$$

$\mathcal{R}_3(O_h)$

$$\begin{aligned}
 G'_{\alpha\gamma} &= \{4G'_{\alpha\gamma} + G''_{\alpha\gamma} | A_1\} + \{G'_{\alpha\gamma} | A_2\} + \{3G'_{\alpha\gamma} + 2G''_{\alpha\gamma} | E\} \\
 G''_{\alpha\gamma} &= \{4G'_{\alpha\gamma} + G''_{\alpha\gamma} | A_1\} + \{G''_{\alpha\gamma} | A_2\} + \{2G'_{\alpha\gamma} + 3G''_{\alpha\gamma} | E\} \\
 G'_{\alpha u} &= \{4G'_{\alpha u} + G''_{\alpha u} | A_1\} + \{G'_{\alpha u} | A_2\} + \{3G'_{\alpha u} + 2G''_{\alpha u} | E\} \\
 G''_{\alpha u} &= \{4G'_{\alpha u} + G''_{\alpha u} | A_1\} + \{G''_{\alpha u} | A_2\} + \{2G'_{\alpha u} + 3G''_{\alpha u} | E\} \\
 E_{1\beta}^3 &= \{2E_{1\beta} | A_1\} + \{E_{1\beta} | E\} \\
 E_{2\beta}^3 &= \{2E_{2\beta} | A_1\} + \{E_{2\beta} | E\} \\
 E_{3\beta}^3 &= \{2E_{3\beta} | A_1\} + \{E_{3\beta} | E\}
 \end{aligned}$$

$$I_\beta^3 = \{2E_{1\beta} + E_{2\beta} + E_{3\beta} + 8I_\beta | A_1\} + \{2E_{1\beta} + E_{2\beta} + E_{3\beta} + 2I_\beta | A_2\} + \{3E_{1\beta} + 2E_{2\beta} + 3E_{3\beta} + 9I_\beta | \mathcal{E}\}$$

$$G_{1\alpha\beta}^3 = \{G_{1\alpha\beta} + 2G_{2\alpha\beta} + 2G_{3\alpha\beta} | A_1\} + \{G_{1\alpha\beta} | A_2\} + \{3G_{1\alpha\beta} + G_{2\alpha\beta} + G_{3\alpha\beta} | \mathcal{E}\}$$

$$G_{2\alpha\beta}^3 = \{G_{1\alpha\beta} + 3G_{2\alpha\beta} + G_{3\alpha\beta} | A_1\} + \{G_{2\alpha\beta} | A_2\} + \{G_{1\alpha\beta} + 3G_{2\alpha\beta} + G_{3\alpha\beta} | \mathcal{E}\}$$

$$G_{3\alpha\beta}^3 = \{G_{1\alpha\beta} + G_{2\alpha\beta} + 3G_{3\alpha\beta} | A_1\} + \{G_{3\alpha\beta} | A_2\} + \{G_{1\alpha\beta} + G_{2\alpha\beta} + 3G_{3\alpha\beta} | \mathcal{E}\}$$

$\mathcal{R}_4(O_\alpha)$

$$G_\alpha^3 = \{G_\alpha + 2K_\alpha | A_1\} + \{G_\alpha | A_2\} + \{3G_\alpha + K_\alpha | \mathcal{E}\}$$

$$K_\alpha^3 = \{6G_\alpha + 12K_\alpha | A_1\} + \{4G_\alpha + 5K_\alpha | A_2\} + \{7G_\alpha + 7K_\alpha | \mathcal{E}\}$$

$$E_\beta^3 = \{2E_\beta | A_1\} + \{E_\beta | \mathcal{E}\}$$

$$G_\beta^3 = \{4E_\beta + 3G_\beta | A_1\} + \{G_\beta | A_2\} + \{2E_\beta + 4G_\beta | \mathcal{E}\}$$

$$I_\beta^3 = \{E_\beta + G_\beta + 7I_\beta | A_1\} + \{2E_\beta + G_\beta + 2I_\beta | A_2\} + \{4E_\beta + 2G_\beta + 9I_\beta | \mathcal{E}\}$$

$$G_{1\alpha\beta}^3 = \{2G_{1\alpha\beta} + G_{2\alpha\beta} + K_{\alpha\beta} | A_1\} + \{G_{1\alpha\beta} | A_2\} + \{2G_{1\alpha\beta} + G_{2\alpha\beta} + K_{\alpha\beta} | \mathcal{E}\}$$

$$G_{2\alpha\beta}^3 = \{G_{1\alpha\beta} + 2G_{2\alpha\beta} + K_{\alpha\beta} | A_1\} + \{G_{2\alpha\beta} | A_2\} + \{G_{1\alpha\beta} + 2G_{2\alpha\beta} + K_{\alpha\beta} | \mathcal{E}\}$$

$$K_{\alpha\beta}^3 = \{4G_{1\alpha\beta} + 4G_{2\alpha\beta} + 11K_{\alpha\beta} | A_1\} + \{2G_{1\alpha\beta} + 2G_{2\alpha\beta} + 5K_{\alpha\beta} | A_2\} + \{7G_{1\alpha\beta} + 7G_{2\alpha\beta} + 14K_{\alpha\beta} | \mathcal{E}\}$$

$\mathcal{R}(I)$

$$E_{\frac{3}{2}}^3 = \{G_{\frac{3}{2}} | A_1\} + \{E_{\frac{3}{2}} | \mathcal{E}\}$$

$$E_{\frac{7}{2}}^3 = \{G_{\frac{3}{2}} | A_1\} + \{E_{\frac{7}{2}} | \mathcal{E}\}$$

$$G_{\frac{3}{2}}^3 = \{2G_{\frac{3}{2}} + 2I_{\frac{3}{2}} | A_1\} + \{G_{\frac{3}{2}} | A_2\} + \{E_{\frac{3}{2}} + E_{\frac{7}{2}} + G_{\frac{3}{2}} + 2I_{\frac{3}{2}} | \mathcal{E}\}$$

$$I_{\frac{3}{2}}^3 = \{E_{\frac{3}{2}} + E_{\frac{7}{2}} + 4G_{\frac{3}{2}} + 6I_{\frac{3}{2}} | A_1\} + \{2G_{\frac{3}{2}} + 2I_{\frac{3}{2}} | A_2\} + \{3E_{\frac{3}{2}} + 3E_{\frac{7}{2}} + 4G_{\frac{3}{2}} + 7I_{\frac{3}{2}} | \mathcal{E}\}$$

$\mathcal{R}_1(I_u)$

$$E_{\frac{1}{2}g}^3 = \{G_{\frac{3}{2}g} | A_1\} + \{E_{\frac{1}{2}g} | \mathcal{E}\}$$

$$E_{\frac{7}{2}g}^3 = \{G_{\frac{3}{2}g} | A_1\} + \{E_{\frac{7}{2}g} | \mathcal{E}\}$$

$$E_{\frac{1}{2}u}^3 = \{G_{\frac{3}{2}u} | A_1\} + \{E_{\frac{1}{2}u} | \mathcal{E}\}$$

$$E_{\frac{7}{2}u}^3 = \{G_{\frac{3}{2}u} | A_1\} + \{E_{\frac{7}{2}u} | \mathcal{E}\}$$

$$G_{\frac{3}{2}g}^3 = \{2G_{\frac{3}{2}g} + 2I_{\frac{3}{2}g} | A_1\} + \{G_{\frac{3}{2}g} | A_2\} + \{E_{\frac{1}{2}g} + E_{\frac{7}{2}g} + G_{\frac{3}{2}g} + 2I_{\frac{3}{2}g} | \mathcal{E}\}$$

$$G_{\frac{3}{2}u}^3 = \{2G_{\frac{3}{2}u} + 2I_{\frac{3}{2}u} | A_1\} + \{G_{\frac{3}{2}u} | A_2\} + \{E_{\frac{1}{2}u} + E_{\frac{7}{2}u} + G_{\frac{3}{2}u} + 2I_{\frac{3}{2}u} | \mathcal{E}\}$$

$$I_{\frac{3}{2}g}^3 = \{E_{\frac{1}{2}g} + E_{\frac{7}{2}g} + 4G_{\frac{3}{2}g} + 6I_{\frac{3}{2}g} | A_1\} + \{2G_{\frac{3}{2}g} + 2I_{\frac{3}{2}g} | A_2\} + \{3E_{\frac{1}{2}g} + 3E_{\frac{7}{2}g} + 4G_{\frac{3}{2}g} + 7I_{\frac{3}{2}g} | \mathcal{E}\}$$

$$I_{\frac{3}{2}u}^3 = \{E_{\frac{1}{2}u} + E_{\frac{7}{2}u} + 4G_{\frac{3}{2}u} + 6I_{\frac{3}{2}u} | A_1\} + \{2G_{\frac{3}{2}u} + 2I_{\frac{3}{2}u} | A_2\} + \{3E_{\frac{1}{2}u} + 3E_{\frac{7}{2}u} + 4G_{\frac{3}{2}u} + 7I_{\frac{3}{2}u} | \mathcal{E}\}$$

$\mathcal{R}_2(I_h)$

$$\begin{aligned} G_{1\alpha}^3 &= \{G_{1\alpha} + 2K_\alpha | A_1\} + \{G_{1\alpha} | A_2\} + \{3G_{1\alpha} + K_\alpha | E\} \\ G_{2\alpha}^3 &= \{G_{2\alpha} + 2K_\alpha | A_1\} + \{G_{2\alpha} | A_2\} + \{3G_{2\alpha} + K_\alpha | E\} \\ K_\alpha^3 &= \{G_{1\alpha} + G_{2\alpha} + 5K_\alpha + 7O_\alpha | A_1\} + \{G_{1\alpha} + G_{2\alpha} + 3K_\alpha + 2O_\alpha | A_2\} + \\ &\quad + \{3G_{1\alpha} + 3G_{2\alpha} + 6K_\alpha + 8O_\alpha | E\} \\ O_\alpha^3 &= \{7G_{1\alpha} + 7G_{2\alpha} + 16K_\alpha + 11O_\alpha | A_1\} + \{6G_{1\alpha} + 6G_{2\alpha} + 14K_\alpha + 8O_\alpha | A_2\} + \\ &\quad + \{16G_{1\alpha} + 16G_{2\alpha} + 30K_\alpha + 17O_\alpha | E\} \end{aligned}$$

$\mathcal{R}_1(K_h)$

$$\begin{aligned} D_{\frac{1}{2}g}^3 &= \{D_{\frac{3}{2}g} | A_1\} + \{D_{\frac{1}{2}g} | E\} \\ D_{\frac{1}{2}u}^3 &= \{D_{\frac{3}{2}u} | A_1\} + \{D_{\frac{1}{2}u} | E\} \\ D_{\frac{3}{2}g}^3 &= \{D_{\frac{3}{2}g} + D_{\frac{5}{2}g} + D_{\frac{7}{2}g} | A_1\} + \{D_{\frac{3}{2}g} | A_2\} + \{D_{\frac{1}{2}g} + D_{\frac{3}{2}g} + D_{\frac{5}{2}g} + D_{\frac{7}{2}g} | E\} \\ D_{\frac{3}{2}u}^3 &= \{D_{\frac{3}{2}u} + D_{\frac{5}{2}u} + D_{\frac{7}{2}u} | A_1\} + \{D_{\frac{3}{2}u} | A_2\} + \{D_{\frac{1}{2}u} + D_{\frac{3}{2}u} + D_{\frac{5}{2}u} + D_{\frac{7}{2}u} | E\} \\ D_{\frac{5}{2}g}^3 &= \{D_{\frac{3}{2}g} + D_{\frac{5}{2}g} + D_{\frac{7}{2}g} + D_{\frac{9}{2}g} + D_{\frac{11}{2}g} + D_{\frac{13}{2}g} | A_1\} + \{D_{\frac{3}{2}g} + D_{\frac{5}{2}g} + D_{\frac{7}{2}g} | A_2\} + \\ &\quad + \{D_{\frac{1}{2}g} + D_{\frac{3}{2}g} + 2D_{\frac{5}{2}g} + 2D_{\frac{7}{2}g} + D_{\frac{9}{2}g} + D_{\frac{11}{2}g} + D_{\frac{13}{2}g} | E\} \\ D_{\frac{5}{2}u}^3 &= \{D_{\frac{3}{2}u} + D_{\frac{5}{2}u} + D_{\frac{7}{2}u} + D_{\frac{9}{2}u} + D_{\frac{11}{2}u} + D_{\frac{13}{2}u} | A_1\} + \{D_{\frac{3}{2}u} + D_{\frac{5}{2}u} + D_{\frac{7}{2}u} | A_2\} + \\ &\quad + \{D_{\frac{1}{2}u} + D_{\frac{3}{2}u} + 2D_{\frac{5}{2}u} + 2D_{\frac{7}{2}u} + D_{\frac{9}{2}u} + D_{\frac{11}{2}u} + D_{\frac{13}{2}u} | E\} \end{aligned}$$

$\mathcal{R}_2(K_h)$

$$\begin{aligned} D_{\frac{1}{2}\alpha}^3 &= \{D_{\frac{1}{2}\alpha} + 2D_{\frac{3}{2}\alpha} | A_1\} + \{D_{\frac{1}{2}\alpha} | A_2\} + \{3D_{\frac{1}{2}\alpha} + D_{\frac{3}{2}\alpha} | E\} \\ D_{\frac{3}{2}\alpha}^3 &= \{D_{\frac{1}{2}\alpha} + 3D_{\frac{3}{2}\alpha} + 3D_{\frac{5}{2}\alpha} + D_{\frac{7}{2}\alpha} + 2D_{\frac{9}{2}\alpha} | A_1\} + \{D_{\frac{1}{2}\alpha} + 3D_{\frac{3}{2}\alpha} + D_{\frac{5}{2}\alpha} + D_{\frac{7}{2}\alpha} | A_2\} + \\ &\quad + \{3D_{\frac{1}{2}\alpha} + 5D_{\frac{3}{2}\alpha} + 4D_{\frac{5}{2}\alpha} + 3D_{\frac{7}{2}\alpha} + D_{\frac{9}{2}\alpha} | E\} \\ D_{\frac{5}{2}\alpha}^3 &= \{D_{\frac{1}{2}\alpha} + 3D_{\frac{3}{2}\alpha} + 4D_{\frac{5}{2}\alpha} + 4D_{\frac{7}{2}\alpha} + 3D_{\frac{9}{2}\alpha} + 3D_{\frac{11}{2}\alpha} + D_{\frac{13}{2}\alpha} + 2D_{\frac{15}{2}\alpha} | A_1\} + \\ &\quad + \{D_{\frac{1}{2}\alpha} + 3D_{\frac{3}{2}\alpha} + 4D_{\frac{5}{2}\alpha} + 2D_{\frac{7}{2}\alpha} + 3D_{\frac{9}{2}\alpha} + D_{\frac{11}{2}\alpha} + D_{\frac{13}{2}\alpha} | A_2\} + \\ &\quad + \{3D_{\frac{1}{2}\alpha} + 5D_{\frac{3}{2}\alpha} + 8D_{\frac{5}{2}\alpha} + 7D_{\frac{7}{2}\alpha} + 5D_{\frac{9}{2}\alpha} + 4D_{\frac{11}{2}\alpha} + 3D_{\frac{13}{2}\alpha} + D_{\frac{15}{2}\alpha} | E\} \end{aligned}$$

Table 4-2.2 The symmetrized cubes of those representations of the representation groups which yield the projective representations of the point groups.

CHAPTER 5

APPLICATION OF THE THEORY OF PROJECTIVE REPRESENTATIONS
IN THE DERIVATION OF THE DOUBLE-VALUED REPRESENTATIONS
OF THE POINT GROUPS AND ALL THE REPRESENTATIONS OF THE
SPACE GROUPS

5.1 DOUBLE-VALUED REPRESENTATIONS

5.1.1 INTRODUCTION

The concept of a double group was introduced by Bethe (14) for consideration of the effects of electron spin. Since if the total angular momentum J has half integral values (i.e. ions with an odd number of electrons) the representations of the rotation group are double-valued. The quantum number j forms a basis for the character of the representation under a given symmetry operation. If J is an integer, the character of the rotation through an angle α is given by

$$\chi(\alpha) = \frac{\sin(j + \frac{1}{2})\alpha}{\sin(\frac{1}{2}\alpha)}$$

Hence $\chi(\alpha) = \chi(\alpha + 2\pi)$ and 2π is the identity operation. However, if J has half-integral values

$$\chi(\alpha + 2\pi) = -\chi(\alpha)$$

hence 4π is now the identity operation. These classes of groups are called the double groups. The definition of a double group given by Opechowski (15) is as follows

The double group G^+ , of a group G of order g , which is a subgroup of $K = O(3)$, the three-dimensional rotation group, is the abstract group of order $2g$ having the same multiplication table as the $2g$ matrices of $K^+ = SU(2)$ which correspond to the elements of the group G . The group $K^+ = SU(2)$ contains all the unitary unimodular matrices in two dimensions.

The representations of G^+ are therefore of two types

1. The single-valued representations where

$$\chi(g_i) = \chi(Rg_i) \quad g_i \in G$$

R rotation through 2π

2. The double-valued representations where

$$\chi(g_i) = -\chi(Rg_i)$$

5.1.2 THE DERIVATION OF THE DOUBLE-VALUED REPRESENTATIONS FROM THE PROJECTIVE REPRESENTATIONS OF THE POINT GROUPS

Projective representations may be used to find the double-valued representations of a group, irrespective of whether the multiplier is of order two. It should be emphasized that whereas the representation group is the extension of G by M , the double group, G^+ , is the extension of C_1^+ by G where C_1^+ is the group consisting of the identity and the element, R , which reverses the sign of the spin functions for systems with an odd number of electrons. Any isomorphism of $R(G)$ and G^+ is therefore accidental rather than inherent. However, it can be shown that a certain class of representations of $R(G)$, which correspond to a class of projective representations of G , can always be modified so that they provide the double-valued representations of G and further that these unique double-valued representations can be obtained from any of the different sets of projective representations corresponding to representation groups. This problem was first discussed by Weyl (20) and subsequently developed by Hurley (35).

The double-valued representations of a group G^+ are defined such that

$$\delta(Rg_i) = -\delta(g_i)$$

where R commutes with all elements g_i of G^+ . This law is also obeyed for the class α of representations of $R(G)$ for which the representative matrices,

$$\Delta(m_\alpha r_i) = -\Delta(r_i)$$

where m_α is an element of the multiplier, since by projection onto G ,

$$\pi(m_\alpha r_i) = g_i \text{ and } \pi(r_i) = g_i \text{ and } \Delta(r_i) = \phi \delta(g_i),$$

where ϕ is a phase factor to be determined.

The double-valued representations are thus identified by the class α of representations of $R(G)$ and their character systems can be determined once the phase factor (known as a gauge transformation in this context) has been found by comparing the relationships between the generating matrices $\{\tilde{P}, \tilde{Q}, \tilde{A}, \tilde{B}\}$ of the group $R(G)$ with those which hold for the double-valued representations of the group G^+ . This will now be illustrated in the case of the dihedral group $G = D_4$.

D_4^+	$R_1(D_4)$	$R_2(D_4)$	$R_3(D_4)$
$\tilde{A}^4 = -\tilde{E}$	$\tilde{P}^4 = \alpha\tilde{E}$	$\tilde{P}^4 = \alpha\tilde{E}$	$\tilde{P}^4 = \alpha\tilde{E}$
$\tilde{B}^2 = -\tilde{E}$	$\tilde{Q}^2 = \alpha\tilde{E}$	$\tilde{Q}^2 = \alpha\tilde{E}$	$\tilde{Q}^2 = \alpha\tilde{E}$
$\tilde{B}\tilde{A} = -\tilde{A}^3\tilde{B}$	$\tilde{Q}\tilde{P} = \alpha\tilde{P}^3\tilde{Q}$	$\tilde{Q}\tilde{P} = \alpha\tilde{P}^3\tilde{Q}$	$\tilde{Q}\tilde{P} = \tilde{P}^3\tilde{Q}$

Required gauge transformation	$P \rightarrow A$	$P \rightarrow A$	$P \rightarrow \frac{1}{2} iA$
	$Q \rightarrow B$	$A \rightarrow \frac{1}{2} iB$	$Q \rightarrow \frac{1}{2} iB$
Required class of representations	$\alpha = -1$	$\alpha = -1$	$\alpha = -1$

The character systems are now derived by effecting the gauge transformations on the elements of a representation group and then dividing the relevant projective characters through by any resulting phase factors to obtain the characters of the double-valued representations of D_4^+ . As an example we choose $R_3(D_4)$. The required projective characters are those of the separably degenerate $G_{1\alpha}$ representation.

$R_3(D_4)$	E	P^4	$\{P\}$	$\{P^5\}$	$\{P^2\}$	$\{Q\}$	$\{PQ\}$
$G_{I\alpha} \begin{cases} G_{I\alpha}^+ \\ G_{I\alpha}^- \end{cases}$	2	-2	$i\sqrt{2}$	$-i\sqrt{2}$	0	0	0
	2	-2	$-i\sqrt{2}$	$i\sqrt{2}$	0	0	0
phase factor $\times D_4^+$	E	A^4	$i\{A\}$	$i\{A^5\}$	$-\{A^2\}$	$i\{B\}$	$-\{AB\}$
$E_{\frac{1}{2}}$	2	-2	$\sqrt{2}$	$-\sqrt{2}$	0	0	0
$E_{\frac{3}{2}}$	2	-2	$-\sqrt{2}$	$\sqrt{2}$	0	0	0

Hence this process has resolved the complex conjugate pair of representations $\{G_{1\alpha}^+, G_{1\alpha}^-\}$ into the real double-valued representations $\{E_{\frac{1}{2}}, E_{\frac{3}{2}}\}$ of D_4^+ . The same representations are obtained as a set if combinations of \pm signs in the phase factors are used. Further, the same representations are similarly obtained from $R_1(D_4)$ and $R_2(D_4)$.

The case of the regular octahedron double group, $O_h^+ = G$, is interesting since it provides the simplest example among the point groups where the double-valued representations are derived from only one class of projective representations. The generating relationships for the matrices corresponding to the elements of the different representation groups are simplified by writing them in terms of matrices of these elements which can be mapped onto matrices of the elements of O_h^+ .

O_h^+	$R_1(O_h)$	$R_2(O_h)$	$R_3(O_h)$	$R_4(O_h)$
	$\tilde{P}^2 = \tilde{Q}^2 = \alpha \tilde{E}$	$\tilde{P}^2 = \tilde{Q}^2 = \alpha \tilde{E}$	$\tilde{P}^2 = \tilde{Q}^2 = \alpha \tilde{E}$	$\tilde{P}^2 = \tilde{Q}^2 = \tilde{T}^2 = \alpha \tilde{E}$
$\tilde{A}^2 = \tilde{B}^2 = \tilde{D}^2 = -\tilde{E}$	$\tilde{S}^2 = \beta \tilde{E}$	$\tilde{R}^3 = \tilde{S}^2 = \tilde{E}$	$\tilde{R}^3 = \tilde{E}$	$\tilde{R}^3 = \tilde{E}$
$\tilde{C}^3 = \tilde{I}^2 = \tilde{E}$	$\tilde{R}^3 = \tilde{T}^2 = \tilde{E}$	$\tilde{T}^2 = \beta \tilde{E}$	$\tilde{S}^2 = \tilde{T}^2 = \beta \tilde{E}$	$\tilde{S}^2 = \beta \tilde{E}$
$\tilde{B}\tilde{A} = -\tilde{A}\tilde{B}$	$\tilde{Q}\tilde{P} = \alpha \tilde{P}\tilde{Q}$	$\tilde{Q}\tilde{P} = \alpha \tilde{P}\tilde{Q}$	$\tilde{Q}\tilde{P} = \alpha \tilde{P}\tilde{Q}$	$\tilde{Q}\tilde{P} = \alpha \tilde{P}\tilde{Q}$
$\tilde{C}\tilde{A} = \tilde{B}\tilde{C}$	$\tilde{R}\tilde{P} = \tilde{Q}\tilde{R}$	$\tilde{R}\tilde{P} = \tilde{Q}\tilde{R}$	$\tilde{R}\tilde{P} = \tilde{Q}\tilde{R}$	$\tilde{R}\tilde{P} = \tilde{Q}\tilde{R}$
$\tilde{C}\tilde{B} = \tilde{A}\tilde{B}\tilde{C}$	$\tilde{R}\tilde{Q} = \tilde{P}\tilde{Q}\tilde{R}$	$\tilde{R}\tilde{Q} = \tilde{P}\tilde{Q}\tilde{R}$	$\tilde{R}\tilde{Q} = \tilde{P}\tilde{Q}\tilde{R}$	$\tilde{R}\tilde{Q} = \tilde{P}\tilde{Q}\tilde{R}$
$\tilde{D}\tilde{A} = -\tilde{B}\tilde{D}$	$\tilde{S}\tilde{P} = \alpha \tilde{Q}\tilde{S}$	$\tilde{S}\tilde{P} = \alpha \tilde{Q}\tilde{S}$	$\tilde{S}\tilde{P} = \alpha \tilde{Q}\tilde{S}$	$\tilde{S}\tilde{P} = \alpha \tilde{Q}\tilde{S}$
$\tilde{D}\tilde{B} = -\tilde{A}\tilde{D}$	$\tilde{S}\tilde{Q} = \alpha \tilde{P}\tilde{S}$	$\tilde{S}\tilde{Q} = \alpha \tilde{P}\tilde{S}$	$\tilde{S}\tilde{Q} = \alpha \tilde{P}\tilde{S}$	$\tilde{S}\tilde{Q} = \alpha \tilde{P}\tilde{S}$
$\tilde{D}\tilde{C} = \tilde{C}^2 \tilde{D}$	$\tilde{S}\tilde{R} = \tilde{R}^2 \tilde{S}$	$\tilde{S}\tilde{R} = \tilde{R}^2 \tilde{S}$	$\tilde{S}\tilde{R} = \tilde{R}^2 \tilde{S}$	$\tilde{S}\tilde{R} = \tilde{R}^2 \tilde{S}$
$\tilde{I}\tilde{A} = \tilde{A}\tilde{I}$	$\tilde{T}\tilde{P} = \tilde{P}\tilde{T}$	$\tilde{T}\tilde{P} = \tilde{P}\tilde{T}$	$\tilde{T}\tilde{P} = \tilde{P}\tilde{T}$	$\tilde{T}\tilde{P} = \tilde{P}\tilde{T}$
$\tilde{I}\tilde{B} = \tilde{B}\tilde{I}$	$\tilde{T}\tilde{Q} = \tilde{Q}\tilde{T}$	$\tilde{T}\tilde{Q} = \tilde{Q}\tilde{T}$	$\tilde{T}\tilde{Q} = \tilde{Q}\tilde{T}$	$\tilde{T}\tilde{Q} = \tilde{Q}\tilde{T}$
$\tilde{I}\tilde{C} = \tilde{C}\tilde{I}$	$\tilde{T}\tilde{R} = \tilde{R}\tilde{T}$	$\tilde{T}\tilde{R} = \tilde{R}\tilde{T}$	$\tilde{T}\tilde{R} = \tilde{R}\tilde{T}$	$\tilde{T}\tilde{R} = \tilde{R}\tilde{T}$
$\tilde{I}\tilde{D} = \tilde{D}\tilde{I}$	$\tilde{T}\tilde{S} = \alpha \beta \tilde{S}\tilde{T}$	$\tilde{T}\tilde{S} = \beta \tilde{S}\tilde{T}$	$\tilde{T}\tilde{S} = \beta \tilde{S}\tilde{T}$	$\tilde{T}\tilde{S} = \beta \tilde{S}\tilde{T}$

Required
gauge
transfor-
mations

$P \rightarrow A$	$P \rightarrow A$	$P \rightarrow A$	$P \rightarrow A$
$Q \rightarrow B$	$Q \rightarrow B$	$Q \rightarrow B$	$Q \rightarrow B$
$R \rightarrow C$	$R \rightarrow C$	$R \rightarrow C$	$R \rightarrow C$
$S \rightarrow D$	$S \rightarrow \dagger i D$	$S \rightarrow \dagger i D$	$S \rightarrow \dagger i D$
$T \rightarrow I$	$T \rightarrow I$	$T \rightarrow I$	$T \rightarrow \dagger i I$

Required
class of
represent-
ations

$\alpha = -1$	$\alpha = -1$	$\alpha = -1$	$\alpha = -1$
$\beta = -1$	$\beta = +1$	$\beta = +1$	$\beta = -1$

The calculation of the double-valued representations then proceeds as in the example of D_4^+ and identical sets of double-valued representations of O_h^+ are obtained from all four representation groups.

5.2 SPACE GROUP REPRESENTATIONS

5.2.1 INTRODUCTION

Every space group describes a particular crystal structure based on one of the fourteen Bravais lattices i.e. a three-dimensional array of mathematical points which satisfy the condition that every one of them is in an environment exactly similar to that of any other lattice point. Every space group G contains a set of pure translations $\{E/t\}$ which form an invariant subgroup of G . This is the group of the translational symmetry operations of the Bravais lattice where

$$R_n = n_1 t_1 + n_2 t_2 + n_3 t_3$$

n_1, n_2, n_3 are integers and t_1, t_2, t_3 the translations of the Bravais lattice. All pure (or primitive) translations are of the form

$$\{e/t\} = \{e/R_n\}$$

where the rotational parts $a_i (i = 1 \dots (G))$ are the elements of the corresponding point group G_0 such that the factor group G/T is isomorphic to G_0 . All elements of G may be represented in terms of the minimal non-primitive translations associated with the rotation a_i , corresponding to glide planes and screw axes.

$$\{a_i/t\} = \{a_i/v(a_i) + R_n\} = \{e/R_n\} \{a_i/v(a_i)\}$$

The space groups where all $v(a_i) = 0$ are the symmorphic space groups of which there are seventy-three. These contain the entire point group as a subgroup. The remaining 157 space groups are called the non-symmorphic space groups.

The reciprocal lattice is now defined where the Brillouin zone is the unit cell. It is specified by the set of reciprocal lattice vectors $\{g_1, g_2, g_3\}$ where

$$g_i t_j = 2\pi \delta_{ij} (i, j = 1, 2, 3)$$

The Brillouin zone can be described by a set of \underline{k} vectors where the points \underline{K}_q of the reciprocal lattice are given by $\underline{K}_q = (q_1 \underline{g}_1, q_2 \underline{g}_2, q_3 \underline{g}_3)$ where $\{q_1, q_2, q_3\}$ are integers.

The holosymmetric point group P of a given crystal system is that point group which contains the largest number of symmetry operations. Given a point \underline{k} of the Brillouin zone there exist certain elements of P which will transform \underline{k} into itself or some equivalent \underline{k} vector. These elements form a subgroup of P called $P(\underline{k})$, the symmetry group of the \underline{k} vectors. For any \underline{k} vector, $P(\underline{k})$ will be a space group which includes the entire group, T , of pure translations.

Koster (47) reduced the problem of determining space group representations to that of determining the representations of $P(\underline{k})$, by proving the following theorem:

Any irreducible representation of the space group G includes an irreducible representation of $P(\underline{k})$ in which the pure translations $\{e/R_n\}$ are represented by the diagonal matrices

$$\exp(-i\underline{k} \cdot \underline{R}_n) I$$

where I is the unit matrix. The converse is also true. The problem can be reduced still further by considering the point group $G_0(\underline{k})$ containing the rotational parts of the elements of $P(\underline{k})$, such that the reduced set $\{G_0(\underline{k})\}$ contains the elements

$$\{g\} = \{g/v(g)\}$$

Let $D(\{g\})$ be an irreducible representation of $P(\underline{k})$. Then for any two elements of $\{G_0(\underline{k})\}$

$$\begin{aligned} D(\{g_i\})D(\{g_j\}) &= D(\{g_i\} \{g_j\}) \\ &= D(\{e/R_n(i,j)\} \{g_i g_j\}) \\ &= D(\{e/R_n(i,j)\})D(\{g_i g_j\}) \\ &= \exp(-i\underline{k} \cdot \underline{R}_n(i,j))D(\{g_i g_j\}) \end{aligned}$$

Hence this set of matrices form a representation of $P(k)$ with factor system, $\exp(-ik \cdot R_n(i,j))$.

For symmorphic space groups all $R_n(i,j) = 0$, therefore the vector representations of $G_o(\underline{k})$ will give the space group representations of $P(k)$. Similarly for points on the interior of the Brillouin zone all elements g_i of $G_o(\underline{k})$ leave \underline{k} invariant and again the vector representations of $G_o(\underline{k})$ lead to the space group representations of $P(k)$. Hurley (35) noticed the above facts that the vector representations of $G_o(\underline{k})$ were sufficient when dealing with points in the interior of the Brillouin zone for non-symmorphic space groups.

Projective representations are required for points on the surface or the exterior of the Brillouin zone in non-symmorphic space groups.

5.2.2 DERIVATION OF SPACE GROUP REPRESENTATIONS

Hurley (35) showed how the space group representations could be derived from his tables of projective representations and it will be shown that the space group representations are uniquely determined, irrespective of which set of projective representations, and hence which representation group, is chosen. However, the erroneous tables published which have been specified in previous chapters, do indeed lead to incorrect space group representations. It will be shown that double-valued space group representations are easily obtainable from the tables of representation groups in chapter 3 .

The first example concerns the point R on the surface of the Brillouin zone of the space group $O_h^2 (\cong Pn3n)$. For this point, $G_o(\underline{k})$ is O_h and a suitable set of generators for this group can be derived from those given by Bradley and Cracknell (36). These are in Seitz notation,

$$\begin{aligned} \tilde{A} &= \{C_{2x} | 000\}, \tilde{B} = \{C_{2y} | 000\}, \tilde{C} = \{C_{31}^+ | 000\}, \tilde{D} = \{C_{2b} | 000\}, \\ \tilde{I} &= \{S_2 | \frac{1}{2} \frac{1}{2} \frac{1}{2}\} \end{aligned}$$

and direct application of Bradley and Cracknell's tables yields the relationship between these generators of P(k). As in section 5.1.2, these are compared with the generating relations of the matrices of the representation group to determine the relevant class of projective representations and also by which phase factors they are to be modified.

P(k)	R ₁ (O _h)	R ₂ (O _h)	R ₃ (O _h)	R ₄ (O _h)
$\tilde{A}^2 = \tilde{B}^2 = \tilde{E}$	$\tilde{P}^2 = \tilde{Q}^2 = \alpha \tilde{E}$	$\tilde{P}^2 = \tilde{Q}^2 = \alpha \tilde{E}$	$\tilde{P}^2 = \tilde{Q}^2 = \alpha \tilde{E}$	$\tilde{P}^2 = \tilde{Q}^2 = \tilde{T}^2 = \alpha \tilde{E}$
$\tilde{C}^3 = \tilde{E}$	$\tilde{S}^2 = \beta \tilde{E}$	$\tilde{R}^3 = \tilde{S}^2 = \tilde{E}$	$\tilde{R}^3 = \tilde{E}$	$\tilde{R}^3 = \tilde{E}$
$\tilde{D}^2 = \tilde{I}^2 = \tilde{E}$	$\tilde{R}^3 = \tilde{T}^2 = \tilde{E}$	$\tilde{T}^2 = \beta \tilde{E}$	$\tilde{S}^2 = \tilde{T}^2 = \beta \tilde{E}$	$\tilde{S}^2 = \beta \tilde{E}$
$\tilde{B}\tilde{A} = \tilde{A}\tilde{B}$	$\tilde{Q}\tilde{P} = \alpha \tilde{P}\tilde{Q}$	$\tilde{Q}\tilde{P} = \alpha \tilde{P}\tilde{Q}$	$\tilde{Q}\tilde{P} = \alpha \tilde{P}\tilde{Q}$	$\tilde{Q}\tilde{P} = \alpha \tilde{P}\tilde{Q}$
$\tilde{C}\tilde{A} = \tilde{B}\tilde{C}$	$\tilde{R}\tilde{P} = \tilde{Q}\tilde{R}$	$\tilde{R}\tilde{P} = \tilde{Q}\tilde{R}$	$\tilde{R}\tilde{P} = \tilde{Q}\tilde{R}$	$\tilde{R}\tilde{P} = \tilde{Q}\tilde{R}$
$\tilde{C}\tilde{B} = \tilde{A}\tilde{B}\tilde{C}$	$\tilde{R}\tilde{Q} = \tilde{P}\tilde{Q}\tilde{R}$	$\tilde{R}\tilde{Q} = \tilde{P}\tilde{Q}\tilde{R}$	$\tilde{R}\tilde{Q} = \tilde{P}\tilde{Q}\tilde{R}$	$\tilde{R}\tilde{Q} = \tilde{P}\tilde{Q}\tilde{R}$
$\tilde{D}\tilde{A} = \tilde{B}\tilde{D}$	$\tilde{S}\tilde{P} = \alpha \tilde{Q}\tilde{S}$	$\tilde{S}\tilde{P} = \alpha \tilde{Q}\tilde{S}$	$\tilde{S}\tilde{P} = \alpha \tilde{Q}\tilde{S}$	$\tilde{S}\tilde{P} = \alpha \tilde{Q}\tilde{S}$
$\tilde{D}\tilde{B} = \tilde{A}\tilde{D}$	$\tilde{S}\tilde{Q} = \alpha \tilde{P}\tilde{S}$	$\tilde{S}\tilde{Q} = \alpha \tilde{P}\tilde{S}$	$\tilde{S}\tilde{Q} = \alpha \tilde{P}\tilde{S}$	$\tilde{S}\tilde{Q} = \alpha \tilde{P}\tilde{S}$
$\tilde{D}\tilde{C} = \tilde{C}^2 \tilde{D}$	$\tilde{S}\tilde{R} = \tilde{R}^2 \tilde{S}$	$\tilde{S}\tilde{R} = \tilde{R}^2 \tilde{S}$	$\tilde{S}\tilde{R} = \tilde{R}^2 \tilde{S}$	$\tilde{S}\tilde{R} = \tilde{R}^2 \tilde{S}$
$\tilde{I}\tilde{A} = \tilde{A}\tilde{I}$	$\tilde{T}\tilde{P} = \tilde{P}\tilde{T}$	$\tilde{T}\tilde{P} = \tilde{P}\tilde{T}$	$\tilde{T}\tilde{P} = \tilde{P}\tilde{T}$	$\tilde{T}\tilde{P} = \tilde{P}\tilde{T}$
$\tilde{I}\tilde{B} = \tilde{B}\tilde{I}$	$\tilde{T}\tilde{Q} = \tilde{Q}\tilde{T}$	$\tilde{T}\tilde{Q} = \tilde{Q}\tilde{T}$	$\tilde{T}\tilde{Q} = \tilde{Q}\tilde{T}$	$\tilde{T}\tilde{Q} = \tilde{Q}\tilde{T}$
$\tilde{I}\tilde{C} = \tilde{C}\tilde{I}$	$\tilde{T}\tilde{R} = \tilde{R}\tilde{T}$	$\tilde{T}\tilde{R} = \tilde{R}\tilde{T}$	$\tilde{T}\tilde{R} = \tilde{R}\tilde{T}$	$\tilde{T}\tilde{R} = \tilde{R}\tilde{T}$
$\tilde{I}\tilde{D} = -\tilde{D}\tilde{I}$	$\tilde{T}\tilde{S} = \alpha \beta \tilde{S}\tilde{T}$	$\tilde{T}\tilde{S} = \beta \tilde{S}\tilde{T}$	$\tilde{T}\tilde{S} = \beta \tilde{S}\tilde{T}$	$\tilde{T}\tilde{S} = \beta \tilde{S}\tilde{T}$

Required gauge transformation	$\left\{ \begin{array}{l} P \rightarrow A \\ Q \rightarrow B \\ R \rightarrow C \\ S \rightarrow \pm i D \\ T \rightarrow I \end{array} \right.$	$P \rightarrow A$	$P \rightarrow A$	$P \rightarrow A$	$P \rightarrow A$
		$Q \rightarrow B$	$Q \rightarrow B$	$Q \rightarrow B$	$Q \rightarrow B$
		$R \rightarrow C$	$R \rightarrow C$	$R \rightarrow C$	$R \rightarrow C$
		$S \rightarrow \pm i D$	$S \rightarrow D$	$S \rightarrow \pm i D$	$S \rightarrow \pm i D$
		$T \rightarrow I$	$T \rightarrow \pm i I$	$T \rightarrow \pm i I$	$T \rightarrow \pm i I$
Required class of representations	$\left\{ \begin{array}{l} \alpha = +1 \\ \beta = -1 \end{array} \right.$	$\alpha = +1$	$\alpha = +1$	$\alpha = +1$	$\alpha = +1$
		$\beta = -1$	$\beta = -1$	$\beta = -1$	$\beta = -1$

Inspection of the appropriate classes of representations and division of the characters by the phase factors resulting from the gauge transformations confirms that the space group representations are unique.

A further example will usefully consider the point L in $O_h^8 [F_d3c]$. The group $G_o(k)$ is D_{3d} and generating matrices for this are suitably chosen as

$$\tilde{A} = \left\{ S_{6I}^- \mid \begin{matrix} \frac{3}{4} & \frac{3}{4} & \frac{3}{4} \end{matrix} \right\} \quad \text{and} \quad \tilde{B} = \left\{ C_{2b} \mid \begin{matrix} \frac{1}{4} & \frac{1}{4} & \frac{1}{4} \end{matrix} \right\}$$

The relations between these generators and those of the representation groups of D_{3d} are compared below:

$P(k)$	$R_I(D_{3d})$	$R_2(D_{3d})$	$R_3(D_{3d})$
$\tilde{A}^6 = \tilde{E}$	$\tilde{P}^6 = \alpha \tilde{E}$	$\tilde{P}^6 = \alpha \tilde{E}$	$\tilde{P}^6 = \tilde{E}$
$\tilde{B}^2 = \tilde{E}$	$\tilde{Q}^2 = \alpha \tilde{E}$	$\tilde{Q}^2 = \tilde{E}$	$\tilde{Q}^2 = \alpha \tilde{E}$
$\tilde{B}\tilde{A} = -\tilde{A}^5\tilde{B}$	$\tilde{Q}\tilde{P} = \alpha\tilde{P}^5\tilde{Q}$	$\tilde{Q}\tilde{P} = \alpha\tilde{P}^5\tilde{Q}$	$\tilde{Q}\tilde{P} = \alpha\tilde{P}^5\tilde{Q}$
Required Gauge Transformations	$\left\{ \begin{array}{l} P \rightarrow \pm iA \\ Q \rightarrow \pm iB \end{array} \right.$	$P \rightarrow \pm iA$	$P \rightarrow A$
Required class of Representations		$Q \rightarrow B$	$Q \rightarrow \pm iB$
		$\alpha = -I$	$\alpha = -I$

In all these cases, and for all choices of \pm signs in the phase factors the same space group representations result.

The final example concerns the double-valued representations of the point R of O_h^2 discussed in the first example. The relations between the generating matrices for $P(k)$ differ from those for the single-valued representations only in the signs of $\tilde{A}^2, \tilde{B}^2, \tilde{B}\tilde{A}, \tilde{D}\tilde{A}$ and $\tilde{D}\tilde{B}$. The appropriate gauge transformations and choices of representations are therefore :

$$R_1(O_h): P \rightarrow A, Q \rightarrow B, R \rightarrow C, S \rightarrow D, T \rightarrow I; \quad \alpha = -I, \beta = -I$$

$$R_2(O_h): P \rightarrow A, Q \rightarrow B, R \rightarrow C, S \rightarrow D, T \rightarrow -I; \quad \alpha = -I, \beta = -I$$

$$R_3(O_h): P \rightarrow A, Q \rightarrow B, R \rightarrow C, S \rightarrow \pm iD, T \rightarrow I \quad \alpha = I, \beta = -I$$

$$R_4(O_h): P \rightarrow A, Q \rightarrow B, R \rightarrow C, S \rightarrow \pm iD, T \rightarrow -I; \quad \alpha = -I, \beta = -I$$

The double-valued space group representations so produced are again unique, irrespective of the choice of representation group.

The projective representations of the space groups, recently discussed by Backhouse and Bradley (40,41) could also be straightforwardly derived from the representation group tables in chapter 3. The advantage of these is that it would allow one to construct the equivalent but different sets of projective representations and hence give greater flexibility for ascending and descending in symmetry.

CHAPTER 6

COREPRESENTATIONS OF MAGNETIC GROUPS

6.1 INTRODUCTION

The theme of the previous three chapters is now extended to the representations of the magnetic groups, called corepresentations. It will be shown that the magnetic groups have both unitary and antiunitary symmetry elements and that a special algebra is needed when dealing with their corepresentations.

When considering the projective representations of the point groups, it was shown that the algebra of the projective representations could largely be avoided by identifying them with the ordinary representations of an abstract group called the representation group. In a similar way the algebra special to corepresentations can be avoided by recognizing them as ordinary representations of abstract groups. This can be applied to both single-valued and double-valued corepresentations.

Symmetry properties may be used to simplify the eigenvalue problem, since if the Hamiltonian is invariant under a group of transformations, the eigenstates may be assigned to irreducible representations of the group. Normally the symmetry elements leave the time-averaged atomic positions and electronic charge density invariant. However, if the crystal possesses unpaired electrons it is possible for the equilibrium state to have a non-vanishing time-averaged magnetic moment density, i.e. the magnetic moment changes sign, as with the case of ferromagnetic, antiferromagnetic and ferrimagnetic crystals. These crystals

may be described by the black and white (or dichromatic) magnetic groups where the operation of time inversion, θ , occurs in half the elements of the group. Paramagnetic and Diamagnetic crystals have a time averaged magnetic moment equal to zero and may be described by the grey magnetic groups where θ is itself a symmetry element of the group.

Shubnikov, (18) introduced the idea of operations of anti-symmetry. This operation may be defined by introducing an extra co-ordinate, s , into the crystal system which has only two possible values. Hence in addition to the ordinary crystal co-ordinates, there is the additional co-ordinate which will for example change colour, black to white, or direction of the magnetic moment parallel or antiparallel, or change the spin of a particle from "spin up" to "spin down".

Tavger and Zaitzev (48) first classified the magnetic point groups and realized their significance in the study of the macroscopic properties of magnetic crystals.

6.2 THE EFFECT OF THE OPERATION OF TIME REVERSAL

Allowing operations of antisymmetry in a group structure now leads to a new series of groups:

TYPE I The ordinary point groups of which 32 are crystallographic.

TYPE II The grey point groups of which 32 are crystallographic.

TYPE III The black and white or magnetic point groups of which 58 are crystallographic.

In type I groups the operation, R, of anti-symmetry is not present. For the grey point groups the extra co-ordinate, s, that has been introduced is allowed to take both of its two values simultaneously so that any operation of the point group, G, leaves s unchanged and R times any operation of G changes both black into white and white into black, again leaving s unchanged. For the grey point groups the structure can be written

$$M = G + RG$$

and since R^2 is the identity and R commutes with all elements, the grey groups are direct product groups of the form

$$M = G \times \{E + R\}$$

In the black and white groups R is not an operation in its own right, but multiplies half of the symmetry operations of G, and so

$$M = H + R(G - H)$$

where H is a halving subgroup of G. It is possible to derive 58 of these crystallographic magnetic groups from the 32 crystallographic point groups, since if G is the full point group of unitary and antiunitary operators and H is the invariant subgroup of unitary operators, the 58 magnetic groups can be found by choosing all possible distinct combinations of G and H, where G has twice as many elements as H.

The operation of antisymmetry, R, can be thought of as changing the direction of the magnetic moment or reversing the direction of an electric current. This concept can be extended to that of time inversion. The origin of the

magnetic moment of an atom can be pictured by considering that the electrons are moving in orbits within the atom. The orbiting electrons are similar to small loops or coils carrying an electric current and therefore produce a magnetic moment. A reversal of the time co-ordinate $t \rightarrow -t$ would cause the electrons to orbit in the opposite sense and therefore reverse the direction of the magnetic moment.

Wigner, (49) showed that this operation of time inversion, θ , is antiunitary and that

$$\theta^2 = +E \text{ for an even number of electrons}$$

$$\theta^2 = -E \text{ for an odd number of electrons.}$$

The operation of time inversion on a wave function, Ψ , may be determined by considering the time-dependent Schrödinger equation

$$H \Psi = i \hbar \frac{\delta \Psi}{\delta t}$$

where H is the Hamiltonian operator.

Taking the complex conjugate of the above expression

$$H \Psi^* = -i \hbar \frac{\delta \Psi^*}{\delta t}$$

$$H \Psi^* = i \hbar \frac{\delta \Psi^*}{\delta (-t)}$$

Therefore the sign of t is reversed if Ψ is changed into its complex conjugate. Hence the effect of the operation of time inversion θ on a wave function Ψ is to produce Ψ^* .

$$\theta \Psi = \Psi^*$$

therefore θ is an antiunitary operator. In ordinary point groups all operations are unitary and hence all representative matrices, A , obey the condition

$$A \tilde{A}^* = 1$$

Wigner (50) showed that if u is a unitary operator of M then it is also linear and if it is an antiunitary operator, a , of M it is antilinear.

6.3 COREPRESENTATIONS OF MAGNETIC GROUPS

The corepresentation representative matrices of these non-unitary magnetic groups do not multiply in the same way as the symmetry operations. The corepresentation matrices, $D^i(u)$ and $D^i(a)$ can be defined such that

$$u \Psi_{\alpha}^i = \sum_{\beta=1}^K D^i(u)_{\beta\alpha} \Psi_{\beta}^i$$

$$a \Psi_{\alpha}^i = \sum_{\beta=1}^K D^i(a)_{\beta\alpha} \Psi_{\beta}^i$$

which leads to the following multiplication rules:

$$D(u_i)D(u_j) = D(u_i u_j)$$

$$D(u) D(a) = D(ua)$$

$$D(a) D^*(u) = D(au)$$

$$D(a_i)D^*(a_j) = D(a_i a_j)$$

where the asterisk denotes complex conjugation.

Two solutions of the above are equivalent if they can be transformed into each other by a unitary matrix, α , such that

$$\overline{D(u)} = \alpha^{-1} D(u) \alpha$$

$$\overline{D(a)} = \alpha^{-1} D(a) \alpha^*$$

The matrix $D(u)$ remains unchanged if $a = \omega 1$ is a multiple of the unit matrix. $D(a)$, however, is multiplied by $\omega^{-1} \omega^* = \omega^2$.

The explicit forms for these corepresentation matrices were obtained by Wigner (50). He found that there were three distinct types of corepresentations. If u is an element of the unitary subgroup H and a is one of the antiunitary operators in M and $\Delta(u)$ is a representation of H , the type of corepresentation of M depends on $\Delta(u)$ and $\bar{\Delta}(u)$, where

$$\bar{\Delta}(u) = \Delta^*(a_0^{-1} u a_0)$$

where a_0 is any antiunitary operator in M . If $\Delta(u)$ and $\bar{\Delta}(u)$ are equivalent it is possible to express $\bar{\Delta}(u)$ in the form

$$\beta^{-1} \Delta(u) \beta$$

where β is a unitary matrix. Two possibilities now arise:

FIRST TYPE $\beta \beta^* = +\Delta(a_0^2)$

$$D(u) = \Delta(u) ; D(a) = \pm \Delta(a a_0^{-1}) \beta$$

SECOND TYPE $\beta \beta^* = -\Delta(a_0^2)$

$$D(u) = \begin{pmatrix} \Delta(u) & 0 \\ 0 & \Delta(u) \end{pmatrix} ; D(a) = \begin{pmatrix} 0 & \Delta(a a_0^{-1}) \beta \\ -\Delta(a a_0^{-1}) \beta & 0 \end{pmatrix}$$

If $\Delta(u)$ and $\bar{\Delta}(u)$ are not equivalent this leads to a third type of corepresentation:

THIRD TYPE

$$D(u) = \begin{pmatrix} \Delta(u) & 0 \\ 0 & \bar{\Delta}(u) \end{pmatrix} ; D(a) = \begin{pmatrix} 0 & \Delta(a a_0) \\ \Delta(a_0^{-1} a)^* & 0 \end{pmatrix}$$

Wigner also pointed out that it does not matter which of the antiunitary operators is chosen to be a_0 .

All that remains is to obtain a method to decide which of the above three cases is applicable for each corepresentation. Dimmock and Wheeler (51) gave a very simple test using the characters of the representations of the unitary subgroup.

Since β and $\Delta^i(u)$ are unitary the $\Delta^i(u)$ matrices will satisfy the normal orthogonality relation

$$\sum_K \Delta^i(u_K)_{lm} \Delta^j(u_K)_{pq}^* = \frac{g}{l_i} \delta_{ij} \delta_{lp} \delta_{mq}$$

where l_i is the dimension of $\Delta^i(u)$ and g the order of H .

Then

$$\begin{aligned} \sum_K \Delta^i(a_K^2)_{ll} &= \sum_K \Delta^i(u_K a_0 u_K a_0)_{ll} \\ &= \sum_K \Delta^i(u_K)_{lm} \Delta^i(a_0^2)_{mr} \Delta^i(a_0^{-1} u_K a_0)_{rl} \end{aligned}$$

For the first two types of corepresentation this summation

$$\begin{aligned} \text{is } \sum_K \Delta^i(u_K)_{rm} \Delta^i(a_0^2)_{mr} \beta_{rp}^{-1*} \Delta^i(u_K)_{pq}^* \beta_{ql}^* \\ &= \frac{g}{l_i} \delta_{lp} \delta_{mq} \Delta^i(a_0^2)_{mr} \beta_{pr} \beta_{ql} \\ &= \frac{g}{l_i} \Delta^i(a_0^2)_{mr} \beta_{lr} \beta_{mr}^* \\ &= \frac{g}{l_i} \Delta^i(a_0^2)_{mr} \Delta^i(a_0^2)_{mr}^* \\ &= \frac{g}{l_i} \Delta^i(a_0^2)_{mr} \Delta^i(a_0^{-1})_{rm} \\ &= \frac{g}{l_i} \Delta^i(E)_{mm} \\ &= \pm g \end{aligned}$$

For the third type this summation is

$$\begin{aligned} & \sum_K \Delta^i(u_K)_{lm} \Delta^i(a_0^2)_{mr} \Delta^i(a_0^{-1} u_K a_0)_{rl} \\ &= \sum_K \Delta^i(u_K)_{lm} \Delta^i(a_0^2)_{mr} \Delta^j(u_K)_{rl}^* \\ &= 0 \end{aligned}$$

Therefore

$$\begin{aligned} \sum_K \chi^i(a_K^2) &= +g \text{ for the first type} \\ &= -g \text{ for the second type} \\ &= 0 \text{ for the third type.} \end{aligned}$$

The corepresentations of the grey magnetic groups are fairly straightforward to determine since a_0 can be chosen to be θ . Then

$$\bar{\Delta}(u) = \Delta^*(\theta^{-1} u \theta) = \Delta^*(u)$$

Hence the following simplifications of corepresentation theory are applied only to the black and white magnetic groups.

6.4 IDENTIFICATION OF COREPRESENTATIONS AS ORDINARY REPRESENTATIONS

For the purposes of identifying corepresentations with the ordinary representations of abstract groups, the corepresentations should be divided into those which derive from real (i.e. 1-dimensional or inseparably-degenerate) irreducible representations of H and those which derive from the imaginary, separably-degenerate, irreducible representations of H. Those deriving from real irreducible representations of H can be constructed from a set of real representative matrices for which $\Delta^*(u) = \Delta(u)$ and hence, whichever of Wigner's types of representations of H is involved, $\bar{\Delta}(u)$

is also real and the representative matrices of M , $D(u)$ and $D(a)$ are real. The associative laws for these matrices therefore reduce to those of ordinary representations of an abstract group isomorphic to M . A convenient realization of such an abstract group is G . Hence in this case the representation of $G \cong M$ are isomorphic with the corepresentations of $M \cong G$.

The corepresentations which derive from imaginary, separably-degenerate, representations of H correspond to the ordinary representations of an abstract group, A , which has a halving subgroup isomorphic to H . If the representative matrices of A are $\delta(u')$, $\delta(a')$, a mapping must be found between the antiunitary elements $\{a\}$ of M and the corresponding elements $\{a'\}$ of A such that the following equations may be satisfied simultaneously.

$$D(a)D^*(u) = D(au) \qquad \delta(a')\delta(u') = \delta(a'u')$$

$$D(a_i)D^*(a_j) = D(a_i a_j) \qquad \delta(a'_i)\delta(a'_j) = \delta(a'_i a'_j)$$

In general a set of such matrices $D(u)$, $D(a)$ will not form a group but a loop unless the set contains the complex conjugate of every matrix. This is because the associative law is only established if $D^*(u_i) = D(u_j)$ [$u_j \in H$] and $D^*(a_K) = D(a_l)$ [$a_l \in \theta(G-H)$]. The condition on the unitary elements is always satisfied since it implies $u_j = u_i^{-1}$ and the inverse of every unitary element is contained in H . However, the conditions on the antiunitary elements is not necessarily satisfied and the representative matrices as formulated by Wigner do not obey this condition for all the black and white magnetic groups. Notwithstanding this, it has been found for

the point groups that Wigner's matrices can be transformed to an equivalent set obeying the condition that the complex conjugate shall lie within the set. A single example of this concerns the corepresentation generated by the E representation of C_4 in the magnetic group C_8/C_4 . The E representation of C_4 is separably degenerate and generates two equivalent real corepresentations of C_8/C_4 in which the respective representative matrices for any given element are complex conjugates. A simple transformation of either by a phase factor of modulus unity on the antiunitary elements yields another equivalent corepresentation which contains the complex conjugate of every representative matrix. The corepresentation can then be identified with an ordinary representation of a group, in fact the E representation of the dihedral group D_4 . The actual matrices are tabulated below:

C_8/C_4	E	C_4	C_2	C_4^3	θC_8	θC_8^3	θC_8^5	θC_8^7
Wigner's $D(E^+)$	$\begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix}$	$\begin{pmatrix} i & 0 \\ 0 & -i \end{pmatrix}$	$\begin{pmatrix} -1 & 0 \\ 0 & -1 \end{pmatrix}$	$\begin{pmatrix} -i & 0 \\ 0 & i \end{pmatrix}$	$\begin{pmatrix} 0 & i \\ 1 & 0 \end{pmatrix}$	$\begin{pmatrix} 0 & -1 \\ -i & 0 \end{pmatrix}$	$\begin{pmatrix} 0 & -i \\ -1 & 0 \end{pmatrix}$	$\begin{pmatrix} 0 & 1 \\ i & 0 \end{pmatrix}$
Wigner's $D(E^-)$	$\begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix}$	$\begin{pmatrix} -i & 0 \\ 0 & i \end{pmatrix}$	$\begin{pmatrix} -1 & 0 \\ 0 & -1 \end{pmatrix}$	$\begin{pmatrix} i & 0 \\ 0 & -i \end{pmatrix}$	$\begin{pmatrix} 0 & -i \\ 1 & 0 \end{pmatrix}$	$\begin{pmatrix} 0 & -1 \\ i & 0 \end{pmatrix}$	$\begin{pmatrix} 0 & i \\ -1 & 0 \end{pmatrix}$	$\begin{pmatrix} 0 & 1 \\ -i & 0 \end{pmatrix}$
Transformed $D(E^+)$	$\begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix}$	$\begin{pmatrix} i & 0 \\ 0 & -i \end{pmatrix}$	$\begin{pmatrix} -1 & 0 \\ 0 & -1 \end{pmatrix}$	$\begin{pmatrix} -i & 0 \\ 0 & i \end{pmatrix}$	$\begin{pmatrix} 0 & \eta^* \\ \eta & 0 \end{pmatrix}$	$\begin{pmatrix} 0 & -\eta \\ \eta^* & 0 \end{pmatrix}$	$\begin{pmatrix} 0 & -\eta^* \\ -\eta & 0 \end{pmatrix}$	$\begin{pmatrix} 0 & \eta \\ \eta^* & 0 \end{pmatrix}$

$$\eta = \exp(i\pi/4); \quad i = \exp(i\pi/2); \quad a_0 = \theta C_8; \quad \beta = 1$$

Another case when it is convenient to transform Wigner's matrices is that when the corepresentation generated is in fact separably-degenerate and yet the representative matrices are not in appropriate diagonal form. Such separable degeneracies are not self-evident from Wigner's formulation and have to be diagnosed by determining the frequency of the totally symmetric corepresentation in the square of the irreducible corepresentation being tested. If this is two rather than one the degeneracy is separable. Another test is to see if Burnside's theorem can be applied to the set of corepresentations by comparing the sums of the squares of the degeneracies with the order of the magnetic group. The simplest example of such an occurrence appears in the magnetic group C_4/C_2 where the corepresentation generated by the B representation of C_2 , which is of Wigner's second type, yields a two-dimensional representation described by the matrices below (Gard and Backhouse, 52):

C_4/C_2	E	C_2	θC_4	θC_2
Wigner's	$\begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix}$	$\begin{pmatrix} -1 & 0 \\ 0 & -1 \end{pmatrix}$	$\begin{pmatrix} 0 & 1 \\ -1 & 0 \end{pmatrix}$	$\begin{pmatrix} 0 & -1 \\ 1 & 0 \end{pmatrix}$
D(B)				
Diagonalized	$\begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix}$	$\begin{pmatrix} -1 & 0 \\ 0 & -1 \end{pmatrix}$	$\begin{pmatrix} i & 0 \\ 0 & -i \end{pmatrix}$	$\begin{pmatrix} -i & 0 \\ 0 & i \end{pmatrix}$
D(B)				

These matrices can be diagonalized by a straightforward canonical transformation to exhibit the separably-degenerate components with their imaginary characters. Such a diagonalization would have considerably simplified the laborious calculation of the symmetrized cube outlined by Gard and Backhouse (52). The symbol \sqrt{i} used by Gard and Backhouse

needs to be used with caution since $(\sqrt{i})^* = \sqrt{-i} = \pm i \sqrt{i}$. However only the lower, negative, sign leads to the correct result $(\sqrt{i})^* = 1/\sqrt{i}$.

The structure of the abstract group, A, generated by the corepresentation matrices does not appear to be determinable in an entirely general way, but certain structures appear when the corepresentations belong to specific types.

When all the corepresentations of M leading to Wigner's first type, as in the magnetic group C_{4v}/C_4 , Wigner's formula produces two corepresentations of M for every representation of H and hence M is a direct product of H with a group of order two, provided that the matrix β is the unit matrix. Examples of this kind occur whenever all the antiunitary elements, $\theta(G-H)$, are two-fold. A chosen element a_0 , of $\theta(G-H)$ will then act as a generator of M such that $M = H + a_0 H$. Hence a correspondence $a_i = u_i a_0$ exists between the unitary and antiunitary elements and $D(a_i) = \pm \Delta(u_i) \beta$ by insertion in Wigner's formula. Hence when $\beta = 1$, $D(a_i) = \pm \Delta(u_i)$ as required for a direct product structure. It should be noted that since the characters of the corepresentations, D, depend on whether the + or - sign is chosen, two group-theoretically inequivalent corepresentations are generated, not one as asserted in the current literature. Indeed, the \pm sign has been omitted in many papers subsequent to Wigner's work. Inclusion of both possibilities enables the corepresentations to satisfy Burnside's theorem. The concept of equivalence defined by Wigner on page 336 of his book (50) referred to the fact that wave functions transforming as either corepresentations of the \pm pair would have

the same energy and that one could not decide physically to which possibility a given wave function should be ascribed.

The corepresentations of C_{4v}/C_4 can now be described as ordinary representations of a group isomorphic to the abstract group $C_4 \times C_2 \cong C_{4h}$. However, since $D(A)$, $\overline{D(A)}$, $D(B)$, and $\overline{D(B)}$ derive from real representations of $H = C_4$, they can also be described as ordinary representations of C_{4v} as explained earlier. This is possible because they are not faithful representations of $M = C_{4v}/C_4$, a fact which is true for all one-dimensional representations (except B of C_2). For simplicity, therefore, the corepresentations of C_{4v}/C_4 have been described in terms of just one group isomorphic to C_{4h} .

However, in the case of the magnetic group, T_d/T , where the corepresentations are also of Wigner's first type, the matrices β are not all trivial and so only the corepresentations $D(A)$, $\overline{D(A)}$, $D(E)$ and $\overline{D(E)}$ can be put into correspondence with the representations of an abstract group isomorphic with the direct product group, T_h . Since the A and T representations of $H = T$ are real, $D(A)$, $\overline{D(A)}$, $D(T)$ and $\overline{D(T)}$ correspond to representations of T_d and hence the corepresentations of T_d/T require two abstract groups for their description in terms of real representations. This has occurred because $D(T)$ and $\overline{D(T)}$ are faithful corepresentations of T_d/T .

When the corepresentations of M belong to either Wigner's first or third types, as in the magnetic groups isomorphic to C_{nh}/C_n ($n \gg 3$), each real representation of H yields an inseparably-degenerate corepresentation of M.

This is diagnostic of a semi-direct product structure for the abstract group A. Since the only real representations of C_{nh}/C_n are one-dimensional, the corepresentations can be described in terms of just one abstract group $A \cong C_{nv}$. However, in the case of the group T_n/T , $D(T)$ and $\overline{D(T)}$ are faithful corepresentations and hence must be described in terms of a semi-direct product group $A \cong T_d$.

The corepresentations for the non-crystallographic as well as the crystallographic black and white magnetic groups have been studied, since the non-crystallographic magnetic groups could be useful due to the existence of quasi-icosahedral structures in complex intermetallic compounds where there are magnetic interactions of non-crystallographic symmetry within the unit cell. The generalization of the magnetic groups into group families is fairly straightforward. the type of corepresentation can easily be found since the structure of all the unitary subgroups, H, which are normal point groups, is well known. All that remains is the generalization of the unitary matrix β . It is found that in most cases β is equal to the unit matrix. The following example is one where β does not equal the unit matrix.

Considering the family of groups D_{4n}/D_{2n} having the following structure:

$P^{4n} = Q^2 = E$	$QP = P^{4n-1}Q$
Unitary Elements	Antiunitary Elements
$1 \ll p \ll n$	$1 \ll p \ll n$
$P^{4n-2p} \quad 0 \ll q \ll 2n-1$	$P^{4n-p} \quad 0 \ll q \ll 2n-1$
$EP^{2p} \quad P^{2q}Q$	$PP \quad P^{2q+1}Q$

a_0 may be chosen to be the antiunitary element PQ. The condition on β is

$$\Delta(u)\beta = \beta\Delta^*(a_0^{-1}ua_0)$$

Hence β must satisfy the following equations

$$\Delta(P^{2p})\beta = \beta\Delta^*(PQP^{2p}PQ) = \beta\Delta^*(P^{4n-2p})$$

$$\Delta(P^{2q}Q)\beta = \beta\Delta^*(PQP^{2q}QPQ) = \beta\Delta^*(P^{4n+2-2q}Q)$$

But the unitary subgroup D_{2n} has all real matrices.

Therefore
$$\Delta(P^{2p})\beta = \beta\Delta(P^{4n-2p})$$

$$\Delta(P^{2q}Q)\beta = \beta\Delta(P^{4n+2-2q}Q)$$

If β is the matrix associated with the element PQ then substitution in the above equations shows that they are satisfied. Hence β will be the matrix.

$$\begin{pmatrix} \cos(\pi/2n) & -\sin(\pi/2n) \\ -\sin(\pi/2n) & -\cos(\pi/2n) \end{pmatrix}$$

The results for the black and white magnetic groups may be summarized in the following table.

Abstract group $A \cong G$

All representations of C_{2nv}/C_{nv} , D_{nd}/C_{nv} , D_{nh}/C_{nv} , D_{2n}/D_n ,
 D_{nd}/D_n , D_{nh}/D_n , D_{2nh}/D_{nd} ,
 D_{2nh}/D_{nh} , C_n/T_d , C_n/O , I_h/I ,
 K_h/K .

Abstract Group $A \cong H \times C_2$

All representations of C_{nv}/C_n , D_n/C_n , D_{nh}/C_{nh} ,
 D_{nd}/S_{2n}

Abstract Group $A \cong H \wedge C_2$

All representations of C_{nh}/C_n , C_{4n-2}/C_{2n-1} ,
 S_{4n-2}/C_{2n-1} , C_{2nh}/S_{2n} ,
 $C_{(4n-2)h}/C_{(2n-1)h}$

Cases where two abstract groups are needed are tabulated below.

BLACK AND WHITE GROUPS M	COREPRESENTATIONS		ABSTRACT GROUP A
	D(A)	D(B)	
C_{4n}/C_{2n}	$D(A)$	$D(B)$	G
S_{4n}/C_{2n}	$\overline{D(A)}$	$D(E_1)$	$H \wedge C_2$
C_{4nh}/C_{2nh}	$D(A_g), \overline{D(A_g)}$	$D(B_g), D(B_u)$	G
	$D(A_u), \overline{D(A_u)}$	$D(E_{1g}), D(E_{1u})$	$H \wedge C_2$
T_h/T	$D(A)$	$D(E)$	$H \wedge C_2$
	$\overline{D(A)}$	$D(T), \overline{D(T)}$	$H \times C_2$
T_d/T	$D(A)$	$D(E), \overline{D(E)}$	$H \times C_2$
O/T	$\overline{D(A)}$	$D(T), \overline{D(T)}$	$H \wedge C_2$
O_h/T_h	$D(A_g)$	$D(E_g), \overline{D(E_g)}$	$H \times C_2$
	$\overline{D(A_g)}$	$D(E_u), \overline{D(E_u)}$	
	$D(A_u)$	$D(T_g), \overline{D(T_g)}$	$H \wedge C_2$
	$\overline{D(A_u)}$	$D(T_u), \overline{D(T_u)}$	

6.5. PROPERTIES OF COREPRESENTATION CHARACTER TABLES.

It has already been mentioned that Burnside's theorem can always be applied to corepresentations, provided that the group-theoretical concept of equivalence for corepresentations of Wigner's first type is used rather than the physical concept be imposed. Character tables are, however, not necessarily square unless a single abstract group A can be defined to describe the corepresentations. The concept of conjugacy class as presently defined can only be described in terms of the elements, and not the corepresentative matrices, of M and hence unless $A \cong M$ the class structure is likely to be disturbed. The elements of M have to be mapped into the

classes of A and then each column of the character table will be different. However, when two abstract groups A are required, the number of classes is greater than that of either abstract group. The columns are all orthogonal in the normal sense as indeed are the rows. The order of each class is a direct division of the order of M. The character table is dependent on the choice of a_0 but different choices only lead to permutations of the classes corresponding to a given column of characters.

6.6 DESCENT IN SYMMETRY

The supergroup-subgroup relationships between the black and white groups have been studied by Ascher and Janner (53). It has now been found, on examination of the relationships between the corepresentations, that provided that all group-theoretically inequivalent corepresentations of Wigner's first type are included, the processes of ascent and descent in symmetry obey Frobenius's reciprocity theorem and behave in every way in a similar manner to ordinary representations. Further evidence for not discarding on physical grounds half of the corepresentations of Wigner's first type is provided by the fact that if only the positive sign in the formula $D(a) = \pm \Delta(a a_0^{-1}) \beta$ is arbitrarily chosen, some descents become impossible when a corepresentation in the supergroup correlates with the corepresentation which would have a negative sign in this defining equation in the subgroup. The converse can also happen. The actual correlation of the corepresentations does depend on the choice of a_0 in each group.

6.7 THE SYMMETRIZED POWERS OF COREPRESENTATIONS

Rules for determining the direct products of corepresentations have been studied by Karavaev (54) and Bradley and Davies (55) and rules for reducing symmetrized powers were established by Gard and Backhouse (52) who related all calculations to the unitary subgroup. They were therefore only able to symmetrize their powers up to unitary equivalence and hence could not solve the problem completely. The approach just described solves this problem completely for all black and white groups whose corepresentations can be described in terms of just one abstract group, A . Knowing the symmetrization of the powers of the ordinary representations of A , the symmetrized powers of the corepresentations of M are determined by correspondence.

As an example of this method, consider the symmetric cube of the corepresentation $D(T_1)$ of the magnetic group O_h/T_h . This corresponds to the T_{1g} representation of O_h and by inspection of Table II of Boyle (27) its symmetric cube is $A_{2g} + 2T_{1g} + T_{2g}$ which corresponds to the reducible corepresentation $D(A_2) + 2D(T_1) + D(T_2)$ of O_h/T_h in agreement with Cracknell and Sedaghat (56). The correspondence thus indicates the possibility of a full character theory, contrary to the indications of Gard and Backhouse (52).

However, when two abstract groups are needed to describe the corepresentations, the symmetrization can only be performed in the intersection of these, viz. the unitary subgroup. No full character theory can then exist in such cases.

6.8 DESCRIPTION OF THE CHARACTER TABLES OF DOUBLE-VALUED COREPRESENTATIONS

It is important to study double-valued corepresentations as well as single-valued ones since the wave function of a particle, which is placed in an environment with the symmetry of one of the magnetic point groups, must belong to one of the single valued corepresentations of that group if it has zero or integer spin and to one of the double-valued corepresentations if it has half odd integer spin.

The double-valued corepresentations of the black and white double groups were discussed by Dimmock and Wheeler (51) and Cracknell and Wong (57). Cracknell and Wong specified to which of Wigner's three types each corepresentation belonged together with the matrix β . The matrix β was specified incorrectly in Table 7 of Cracknell and Wong and again in the notes to Table 7.15 of Bradley and Cracknell (36) for those cases where it was claimed to equal the unlikely matrix

$$\chi = \pm \frac{1}{2\sqrt{6}} \begin{pmatrix} (\sqrt{3} + 1) + i(\sqrt{3}-1) & 4i \\ 4i & (\sqrt{3}+1) - i(\sqrt{3}-1) \end{pmatrix}$$

where it should have been $\pm \sigma^* = \pm \begin{pmatrix} 1 & 1+i & 0 \\ \sqrt{2} & 0 & 1-i \end{pmatrix}$ for the

representation $E_{\frac{1}{2}}$ and $\begin{pmatrix} 0 & -i \\ -i & 0 \end{pmatrix}$ for the representation $G_{3/2}$.

There are also two errors in the Cayley table for O' (Table 6.2(a) of Bradley and Cracknell) where $C_{2a} C_{4y}^-$ should equal C_{32}^- and $C_{2a} C_{4x}^+$ should equal C_{32}^+ and not as printed. Also in table 6.1 of Bradley and Cracknell (which specifies the matrices of $SU(2)$ corresponding to the point group O') the

matrix C_{32}^- should read $\frac{1}{2} \begin{pmatrix} 1-i & 1-i \\ -1-i & 1+i \end{pmatrix}$

Since double-valued representations are merely ordinary representations of an extended group, double valued corepresentations are just corepresentations of an extended black and white group and hence no modification of Wigner's (50) formulae is required to determine them. Wigner had already noted that $\Delta(\theta^2) = -1$ for systems with an odd number of electrons viz. the systems where double-valued representations are necessary. The results for the character tables of these double-valued corepresentations show that they can be conveniently derived from one or two abstract groups, A, as summarized in the following table.

Abstract Group $A \cong G$

All representations of C'_{4nv} / C'_{2nv} , D'_{2nd} / C'_{2nv} , D'_{2nd} / D'_{2n} , D'_{4n} / D'_{2n} , O'_h / O' , O'_h / T'_d , I'_h / I' , K'_h / K'

Abstract Group $A \cong H \times C_2$

All representations of C'_{nv} / C'_n , $C'_{(4n-2)v} / C'_{(2n-1)v}$, D'_n / C'_n , D'_{nh} / C'_{nh} , D'_{nh} / C'_{nv} , $D'_{(2n+1)d} / C'_{(2n+1)v}$, D'_{4n+2} / D'_{2n+1} , $D'_{(2n+1)d} / D'_{2n+1}$, D'_{nh} / D'_n , D'_{2nh} / D'_{nd} , D'_{2nh} / D'_{nh} , $D'_{(4n+2)h} / D'_{(2n+1)d}$, D'_{nd} / S'_{2n}

Abstract Group $A \cong H \wedge C_2$

All representations of C'_{nh} / C'_n , C'_{2n} / C'_n , S'_{4n-2} / C'_{2n-1} , C'_{2nh} / S'_{2n} , C'_{2nh} / C'_{nh}

Cases where two abstract groups are needed are tabulated below.

Black and White Groups, M'	Corepresentations	Abstract Group A
T'_h / T'	$D(E_{1/2}), \overline{D(E_{1/2})}$	G
	$D(G_{3/2})$	$H \wedge C_2$
O'_d / T'	$D(E_{1/2}), \overline{D(E_{1/2})}$	G
T'_d / T'	$D(G_{3/2})$	$H \times C_2$
O'_h / T'_h	$D(E_{1/2g}), \overline{D(E_{1/2g})}$	G
	$D(E_{1/2u}), \overline{D(E_{1/2u})}$	
	$D(G_{3/2g}), \overline{D(G_{3/2g})}$	$H \times C_2$
	$D(G_{3/2u}), \overline{D(G_{3/2u})}$	

The character tables for the single-valued and double-valued corepresentations are given in the next section. The two sets of tables could not be conveniently coalesced because the isomorphisms between the black and white groups are changed on extending to the double groups and because it would be necessary to superimpose the different set of relationships between the generating matrices.

6.9 Single-valued and Double-valued Corepresentation Character Tables

S_{4n-2}/C_{2n-1} C_{4n-2}/C_{2n-1} $C_{(2n-1)h}/C_{2n-1}$	$1 \leq p \leq n-1$			$0 \leq q \leq 2n-2$ $A^q B$	$\tilde{A}^{2n-1} = \tilde{E}$ $\tilde{B}^2 = \tilde{E}$ $\tilde{B} \tilde{A} = \tilde{A}^{-2n-2} \tilde{B}$	$\alpha_0 = B$ $\beta = 1$
	E	A^p				
$D(A)$	1	1	1			
$\overline{D(A)}$	1	1	-1			
$1 \leq l \leq n-1; D(E_l)$	2	$2 \cos 2pl\pi/2n-1$	0			
S_{4n-2}/C_{2n-1} C_{4n-2}/C_{2n-1} $C_{(2n-1)h}/C_{2n-1}$					$\tilde{A} = C_{2n-1} ; \tilde{B} = \theta S_2$ $\tilde{A} = C_{2n-1} ; \tilde{B} = \theta C_2$ $\tilde{A} = C_{2n-1} ; \tilde{B} = \theta \sigma_h$	

n odd; C_{2nh}/C_{nh} C_{2nh}/S_{2n} C_{2nh}/C_{2n}	$1 \leq p \leq \frac{1}{2}(n+1)$ $A^{2n-2p+1}$ A^{2p-1} E	$1 \leq p \leq \frac{1}{2}n$ A^{2n-2p} A^{2p}	$0 \leq q \leq n-1$ $A^{2q}B$	$0 \leq q \leq n-1$ $A^{2q+1}B$	$\tilde{A} = \tilde{E}$ $\tilde{B} = \tilde{E}$ $\tilde{B}\tilde{A} = \tilde{A}^{2n-1}\tilde{B}$	$\alpha_0 = B$ $\beta = 1$
D(A)	1	1	1	1		
D(B)	1	1	1	1		
$\overline{D(A)}$	1	1	-1	-1		
$\overline{D(B)}$	1	1	-1	-1		
$1 \leq \ell \leq n-1$; D(E $_{\ell}$)	2	$2 \cos(2p-1)\ell\pi/n$	$2 \cos 2p\ell\pi/n$	0	0	
n odd; C_{2nh}/C_{nh} C_{2nh}/S_{2n} C_{2nh}/C_{2n}	$\tilde{A} = S_n^{2n-1}; \tilde{B} = \theta S_2$ $\tilde{A} = S_{2n}; \tilde{B} = \theta S_2$ (n even) $\tilde{A} = C_{2n}; \tilde{B} = \theta S_2$ (n odd)					

D_{nd}/S_{2n} n odd; D_{nh}/C_{nh} D_{2n}/C_{2n} C_{2nv}/C_{2n}	$1 \leq p \leq 2n-1$ E A^p	$A^p B$	$\tilde{A} = \tilde{B}$ $\tilde{B} = \tilde{E}$ $\tilde{B} \tilde{A} = \tilde{A} \tilde{B}$ $\alpha_c = B$ $\beta = 1$
$D(A)$ $D(B)$ $D(A)$ $D(B)$ $D(E_l)$ $D(E_l)$ $D(E_l)$ $D(E_l)$	1 $(-1)^p$ 1 $(-1)^p$ $\exp(i\pi p/n)$ $\exp(-i\pi p/n)$ $\exp(i\pi p/n)$ $\exp(-i\pi p/n)$	1 $(-1)^p$ 1 $(-1)^{p+1}$ $\exp(i\pi p/n)$ $\exp(-i\pi p/n)$ $-\exp(i\pi p/n)$ $-\exp(-i\pi p/n)$	
D_{nd}/S_{2n} n odd; D_{nh}/C_{nh} D_{2n}/C_{2n} C_{2nv}/C_{2n}		$\tilde{A} = S_{2n}^{2n-1}$; $\tilde{B} = \theta C_2$ $\tilde{A} = S_n^{n-1}$; $\tilde{B} = \theta C_2'$ $\tilde{A} = C_{2n}$; $\tilde{B} = \theta C_2$ $\tilde{A} = C_{2n}$; $\tilde{B} = \theta C_2'$	

$D_{(2n-1)h} / D_{2n-1}$ $D_{(2n-1)d} / D_{2n-1}$ D_{4n-2} / D_{2n-1} $D_{(2n-1)h} / C_{(2n-1)v}$ $D_{(2n-1)d} / C_{(2n-1)v}$ $C_{(4n-2)v} / C_{(2n-1)v}$	$D(A_1)$ $D(A_2)$ $D(A_1)$ $D(A_2)$ $D(E_\theta)$ $D(E_\theta)$	E 	$1 \leq p \leq 2n-1$ A^{4n-2-p} A^p	$0 \leq q \leq 2n-2$ $A^{2q}B$ $A^{2q+1}B$	$\tilde{A}^{4n-2} \tilde{E}$ $\tilde{B}^2 \tilde{E}$ $\tilde{B} \tilde{A} = \tilde{A}^{4n-3} \tilde{B}$ $\alpha_0 = A^3$ $\beta = 1$
$D_{(2n-1)h} / D_{2n-1}$ $D_{(2n-1)d} / D_{2n-1}$ D_{4n-2} / D_{2n-1} $D_{(2n-1)h} / C_{(2n-1)v}$ $D_{(2n-1)d} / C_{(2n-1)v}$ $C_{(4n-2)v} / C_{(2n-1)v}$	$D(A_1)$ $D(A_2)$ $D(A_1)$ $D(A_2)$ $D(E_\theta)$ $D(E_\theta)$	E 	$1 \leq p \leq 2n-1$ A^{4n-2-p} A^p	$0 \leq q \leq 2n-2$ $A^{2q}B$ $A^{2q+1}B$	$\tilde{A}^{4n-2} \tilde{E}$ $\tilde{B}^2 \tilde{E}$ $\tilde{B} \tilde{A} = \tilde{A}^{4n-3} \tilde{B}$ $\alpha_0 = A^3$ $\beta = 1$

D_{2nd}/D_{2n} D_{4n}/D_{2n} D_{2nd}/C_{2nV} C_{4nV}/C_{2nV}	$1 \leq p \leq 2n$ A^{4n-p} A^p	$0 \leq q \leq 2n-1$ $A^{2q}B$	$0 \leq q \leq 2n-1$ $A^{2q+1}B$	$\tilde{A} = \tilde{E}$ $\tilde{B} = \tilde{E}$ $\tilde{B}\tilde{A} = \tilde{A}^{4n-1}\tilde{B}$	$\alpha_3 = AB$
$D(A_1)$	1	1	1	} $\beta = 1$	
$D(A_2)$	$(-1)^p$	-1	1		
$\overline{D(A_1)}$	$(-1)^p$	1	-1	} $\beta = \begin{pmatrix} \cos \pi/2n & -\sin \pi/2n \\ -\sin \pi/2n & -\cos \pi/2n \end{pmatrix}$	
$\overline{D(A_2)}$	1	-1	1		
$D(B)$	$2 \cos p\pi/2$	0	0		
$D(E_0)$	$2 \cos l p\pi/2n$	0	0		
$D(E_i)$	$(-1)^p 2 \cos l p\pi/2n$	0	0		
D_{2nd}/D_{2n} D_{4n}/D_{2n} D_{2nd}/C_{2nV} C_{4nV}/C_{2nV}				$\tilde{A} = \theta S_{4n-1}^n$; $\tilde{B} = C_1^2$ $\tilde{A} = \theta C_{4n}^n$; $\tilde{B} = C_2^2$ $\tilde{A} = \theta S_{4n-1}^n$; $\tilde{B} = \alpha_V$ $\tilde{A} = \theta C_{4n}^n$; $\tilde{B} = \alpha_V$	

D_{2nh}/C_{2nh}	E	$1 \leq p \leq 2n-1$	$0 \leq p \leq 2n-1$	$0 \leq p \leq 2n-1$	$0 \leq p \leq 2n-1$	$\tilde{A}^{2n} = \tilde{B}^2 = \tilde{C}^2 = \tilde{E}$ $\tilde{B}\tilde{A} = \tilde{A}\tilde{B};$ $\tilde{C}\tilde{A} = \tilde{A}\tilde{C}; \tilde{C}\tilde{B} = \tilde{B}\tilde{C}$	$\alpha_0 = C$ $\beta = 1$
		A^p	$A^p B$	$A^p C$	$A^p BC$		
$D(A_g)$	1	1	1	1	1	1	
$D(B_g)$	1	$(-1)^p$	$(-1)^p$	$(-1)^p$	$(-1)^p$	$(-1)^p$	
$D(A_u)$	1	1	1	1	1	1	
$D(B_u)$	1	$(-1)^p$	$(-1)^{p+1}$	$(-1)^p$	$(-1)^{p+1}$	$(-1)^{p+1}$	
$D(A_g)$	1	1	1	1	1	1	
$D(B_g)$	1	$(-1)^p$	$(-1)^p$	$(-1)^{p+1}$	$(-1)^{p+1}$	$(-1)^{p+1}$	
$D(A_u)$	1	1	1	1	1	1	
$D(B_u)$	1	$(-1)^p$	$(-1)^{p+1}$	$(-1)^p$	$(-1)^{p+1}$	$(-1)^{p+1}$	
$1 \leq l \leq n-1; D(E_{1l})$	1	$\exp(i l p \pi / n)$	$\exp(i l p \pi / n)$	$\exp(i l p \pi / n)$	$\exp(i l p \pi / n)$	$\exp(i l p \pi / n)$	
$1 \leq l \leq n-1; D(E_{2l})$	1	$\exp(-i l p \pi / n)$	$\exp(-i l p \pi / n)$	$\exp(-i l p \pi / n)$	$\exp(-i l p \pi / n)$	$\exp(-i l p \pi / n)$	
$1 \leq l \leq n-1; D(\overline{E_{1l}})$	1	$\exp(i l p \pi / n)$	$\exp(-i l p \pi / n)$	$\exp(i l p \pi / n)$	$\exp(-i l p \pi / n)$	$\exp(i l p \pi / n)$	
$1 \leq l \leq n-1; D(\overline{E_{2l}})$	1	$\exp(-i l p \pi / n)$	$\exp(i l p \pi / n)$	$\exp(-i l p \pi / n)$	$\exp(i l p \pi / n)$	$\exp(-i l p \pi / n)$	
D_{2nh}/C_{2nh}							$\tilde{A} = C_{2n}; \tilde{B} = S_2$ $\tilde{C} = \sigma_{C_2}$

$\frac{S_{4n}}{C_{4n}} / \frac{C_{2n}}{C_{2n}}$ $\frac{S_{4n}}{C_{4n}} / \frac{C_{2n}}{C_{2n}}$	E $1 \leq p \leq n$ A_{4n-2p}^{4n-2p} A_{2p}^{2p}	$0 \leq q \leq n-1$ A_{4q+1}^{4q+1}	$0 \leq q \leq n-1$ A_{4q+3}^{4q+3}	$\alpha_0 = A; \beta = 1$
$D(A)$	1	1	1	$\tilde{A} = E$
$\overline{D(A)}$	1	1	-1	
$D(B)$	1	$(-1)^p$	i	$\tilde{A} = E$
$D(B)$	1	$(-1)^p$	$-i$	
$1 \leq l \leq n-1; D(E_l)$	2	$2 \cos(p\pi/n)$	0	$\tilde{B} = \tilde{C} = E; \tilde{A} = \tilde{B}$ $\tilde{C} \tilde{B} = \tilde{B}^{2n-1} \tilde{C}$
$\frac{C_{4n}}{C_{4n}} / \frac{C_{2n}}{C_{2n}}$	S_{4n}	C_{4n}	C_{2n}	$\tilde{A} = \theta C_{4n}; \tilde{B} = C_{2n}; \tilde{C} = \theta C_{4n}$ $\tilde{A} = \theta S_{4n}; \tilde{B} = C_{2n}; \tilde{C} = \theta S_{4n}$

D_{2nh}/D_{nh} D_{2nh}/D_{nd} D_{2nh}/C_{2nv} D_{2nh}/D_{2n}	$1 \leq p \leq n$				$0 \leq p \leq n$			$\tilde{A}^{2n} = \tilde{B}^2 = \tilde{C}^2 = \tilde{E}$ $\tilde{B}\tilde{A} = \tilde{A}^{2n-1}\tilde{B}$ $\tilde{C}\tilde{A} = \tilde{A}\tilde{C}$ $\tilde{C}\tilde{B} = \tilde{B}\tilde{C}$	$a_0 = C$ $\beta = 1$
	E	A^{2n-p} A^p	$0 \leq q \leq n-1$ $A^{2q}B$	$0 \leq q \leq n-1$ $A^{2q+1}B$	$A^{2n-p}C$ A^pC	$0 \leq q \leq n-1$ $A^{2q}BC$	$0 \leq q \leq n-1$ $A^{2q+1}BC$		
$D(A_1)$	1	1	1	1	1	1	1		
$D(A_2)$	1	1	-1	-1	1	-1	-1		
$D(B_1)$	1	$(-1)^p$	1	-1	$(-1)^p$	1	-1		
$D(B_2)$	1	$(-1)^p$	-1	1	$(-1)^p$	-1	1		
$\overline{D(A_1)}$	1	1	1	1	-1	-1	-1		
$\overline{D(A_2)}$	1	1	-1	-1	-1	1	1		
$\overline{D(B_1)}$	1	$(-1)^p$	1	-1	$(-1)^{p+1}$	-1	1		
$\overline{D(B_2)}$	1	$(-1)^p$	-1	1	$(-1)^{p+1}$	1	-1		
$1 \leq l \leq n-1; D(E_l)$	2	$2 \cos p\pi/n$	0	0	$2 \cos p\pi/n$	0	0		
$1 \leq l \leq n-1; \overline{D(E_l)}$	2	$2 \cos p\pi/n$	0	0	$-2 \cos p\pi/n$	0	0		
D_{2nh}/D_{nh} D_{2nh}/D_{nd} D_{2nh}/C_{2nv} D_{2nh}/D_{2n}								$\tilde{A} = S_n^{n-1}; \tilde{B} = C_2'; \tilde{C} = \theta S_2$ $\tilde{A} = S_{2n}^{2n-1}; \tilde{B} = C_2'; \tilde{C} = \theta C_2$ $\tilde{A} = C_{2n}; \tilde{B} = \sigma_d; \tilde{C} = \theta S_2$ $\tilde{A} = C_{2n}; \tilde{B} = C_2'; \tilde{C} = \theta S_2$	

C_{4nh}/C_{2nh}	E	$1 \leq p \leq n$ A^{4n-2p}	$0 \leq q \leq n-1$ A^{4q+1}	$0 \leq q \leq n-1$ A^{4q+3}	$0 \leq p \leq n$ $A^{2p}B$	$0 \leq q \leq n-1$ $A^{4q+1}B$	$0 \leq q \leq n-1$ $A^{4q+3}B$	$\alpha_0 = A; \beta = 1$
$D(A_g)$	1	1	1	1	1	1	1	$\left. \begin{aligned} \tilde{A} &= A \\ \tilde{B} &= B \\ \tilde{C} &= C \\ \tilde{D} &= D \\ \tilde{E} &= E \\ \tilde{F} &= F \end{aligned} \right\}$
$D(A_u)$	1	1	1	1	-1	-1	-1	
$\overline{D(A_g)}$	1	1	-1	-1	1	1	1	
$\overline{D(A_u)}$	1	1	-1	-1	-1	-1	-1	
$D(B_g^+)$	1	$(-1)^p$	i	-i	$(-1)^p$	i	-i	
$D(B_g^-)$	1	$(-1)^p$	-i	i	$(-1)^p$	-i	i	
$D(B_u^+)$	1	$(-1)^p$	i	-i	$(-1)^{p+1}$	-i	i	
$D(B_u^-)$	1	$(-1)^p$	-i	i	$(-1)^{p+1}$	i	-i	
$1 \leq l \leq n-1; D(E_{4l})$	2	$2 \cos l\pi/n$	0	0	$2 \cos 2l\pi/n$	0	0	
$1 \leq l \leq n-1; D(E_{2l})$	2	$2 \cos l\pi/n$	0	0	$-2 \cos l\pi/n$	0	0	
C_{4nh}/C_{2nh}								$\left. \begin{aligned} \tilde{A} &= \theta C_{4n}; \tilde{B} = S_2 \\ \tilde{C} &= C_{2n}; \tilde{D} = S_2 \\ \tilde{E} &= \theta C_{4n} \end{aligned} \right\}$

$\frac{D_{2n-1}/C_{2n-1}}{C_{(2n-1)\nu}/C_{2n-1}}$ E	$1 \leq p \leq 2n-2$ E	$0 \leq p \leq 2n-2$ A^p	$\tilde{A}^{2n-1} = \tilde{E}$ $\tilde{B}^2 = \tilde{E}$ $\tilde{B}\tilde{A} = \tilde{A}\tilde{B}$ $\alpha = \beta$ $\beta = 1$
$D(A)$ $\overline{D(A)}$	$ $ $ $	$ $ $ $	$ $ $-$
$1 \leq l \leq n-1;$ $D(E_l)$ $\overline{D(E_l)}$	$ $ $ $	$\exp(2i\pi lp/2n-1)$ $\exp(-2i\pi lp/2n-1)$	$\exp(2i\pi lp/2n-1)$ $\exp(-2i\pi lp/2n-1)$
$1 \leq l \leq n-1;$ $\overline{D(E_l)}$ $D(E_l)$	$ $ $ $	$\exp(2i\pi lp/2n-1)$ $\exp(-2i\pi lp/2n-1)$	$-\exp(2i\pi lp/2n-1)$ $-\exp(-2i\pi lp/2n-1)$
$\frac{D_{2n-1}/C_{2n-1}}{C_{(2n-1)\nu}/C_{2n-1}}$			$\tilde{A} = C_{2n-1}; \tilde{B} = \theta C_2$ $\tilde{A} = C_{2n-1}; \tilde{B} = \theta \sigma_D$

T_h/T	E	ABC, BC ² AC, ABC ² BC, AC ² C, C ²	AB B A	D	ABCD, BC ² D ACD, ABC ² D BCD, AC ² D CD, C ² D	ABD BD AD	$\alpha_0 = D$ $\beta = 1$
D(A)	1	1	1	1	1	1	$\tilde{A}^2 = \tilde{B}^2 = \tilde{C}^2 = \tilde{D}^2 = \tilde{E}$ $\tilde{B}\tilde{A} = \tilde{A}\tilde{B}; \tilde{C}\tilde{A} = \tilde{B}\tilde{C}$ $\tilde{C}\tilde{B} = \tilde{A}\tilde{B}\tilde{C}; \tilde{D}\tilde{A} = \tilde{A}\tilde{D}$ $\tilde{D}\tilde{E} = \tilde{B}\tilde{D}; \tilde{D}\tilde{C} = \tilde{C}\tilde{D}$ $\tilde{A}^2 = \tilde{B}^2 = \tilde{C}^2 = \tilde{D}^2 = \tilde{E}; \tilde{D}\tilde{A} = \tilde{B}\tilde{D}; \tilde{D}\tilde{B} = \tilde{A}\tilde{D}$ $\tilde{B}\tilde{A} = \tilde{A}\tilde{B}; \tilde{C}\tilde{A} = \tilde{B}\tilde{C}; \tilde{C}\tilde{B} = \tilde{A}\tilde{B}\tilde{C}; \tilde{D}\tilde{C} = \tilde{C}^2\tilde{D}$
$\overline{D(A)}$	1	1	1	-1	-1	-1	
D(T)	3	0	-1	3	0	-1	
$\overline{D(T)}$	3	0	-1	-3	0	-1	
D(E)	2	-1	2	0	0	0	
T_h/T							$\tilde{A} = C_{2x}$ $\tilde{B} = C_{2y}$ $\tilde{C} = C_3$ $\tilde{D} = \theta S_2$

O_k/Γ_h	ABC	BC ²	BC ³	8C ³ I	ABCI	AD, BD	BC ² D, ABC ² D	ACD, ABCD	ACD ² , ABCD ²	ACD ³ , ABCD ³	AD ² , BDI, ABC ² DI	BC ² DI, ABC ² DI	ACDI, ABCDI	AC ² DI, BC ² DI	AC ³ DI, BC ³ DI
$D(A_9)$	1	1	1	1	1	1	1	1	1	1	1	1	1	1	1
$D(A_{10})$	1	1	1	-1	-1	1	1	1	1	1	-1	-1	-1	-1	-1
$D(A_{11})$	1	1	1	1	1	-1	-1	-1	-1	-1	-1	-1	-1	-1	-1
$D(A_{12})$	1	1	1	-1	-1	1	1	1	1	1	1	1	1	1	1
$D(\Gamma_3)$	3	0	0	-3	0	1	1	1	1	1	1	1	1	1	1
$D(\Gamma_4)$	3	0	0	-3	0	1	1	1	1	1	-1	-1	-1	-1	-1
$D(\Gamma_5)$	3	0	0	-3	0	1	1	1	1	1	-1	-1	-1	-1	-1
$D(\Gamma_6)$	3	0	0	-3	0	1	1	1	1	1	1	1	1	1	1
$D(E_9)$	1	ϵ^*	ϵ	1	ϵ	1	ϵ^*	ϵ	ϵ^*	ϵ	1	ϵ^*	ϵ	ϵ^*	ϵ
$D(E_{10})$	1	ϵ	ϵ^*	1	ϵ^*	1	ϵ	ϵ^*	ϵ	ϵ^*	1	ϵ	ϵ^*	ϵ	ϵ^*
$D(E_{11})$	1	ϵ^*	ϵ	-1	ϵ^*	1	ϵ^*	ϵ	ϵ^*	ϵ	-1	ϵ^*	ϵ	-1	ϵ^*
$D(E_{12})$	1	ϵ	ϵ^*	-1	ϵ	1	ϵ	ϵ^*	ϵ	ϵ^*	-1	ϵ	ϵ^*	-1	ϵ
$D(E_{13})$	1	ϵ^*	ϵ	1	ϵ^*	1	ϵ^*	ϵ	ϵ^*	ϵ	-1	ϵ^*	ϵ	-1	ϵ^*
$D(E_{14})$	1	ϵ	ϵ^*	1	ϵ	1	ϵ	ϵ^*	ϵ	ϵ^*	-1	ϵ	ϵ^*	-1	ϵ
$D(E_{15})$	1	ϵ^*	ϵ	-1	ϵ^*	1	ϵ^*	ϵ	ϵ^*	ϵ	-1	ϵ^*	ϵ	-1	ϵ^*
$D(E_{16})$	1	ϵ	ϵ^*	-1	ϵ	1	ϵ	ϵ^*	ϵ	ϵ^*	-1	ϵ	ϵ^*	-1	ϵ

$Q_3 = A_3 B_3 D_3$

$\hat{A} = \hat{B} = \hat{C} = \hat{D} = \hat{I} = \hat{E}$
 $\hat{B}\hat{A} = \hat{A}\hat{B}; \hat{C}\hat{A} = \hat{B}\hat{C}$
 $\hat{C}\hat{B} = \hat{A}\hat{B}\hat{C}; \hat{D}\hat{A} = \hat{B}\hat{D}$
 $\hat{D}\hat{B} = \hat{A}\hat{D}; \hat{D}\hat{C} = \hat{C}\hat{D}$
 $\hat{I}\hat{A} = \hat{A}\hat{I}; \hat{I}\hat{B} = \hat{B}\hat{I}$
 $\hat{I}\hat{C} = \hat{C}\hat{I}; \hat{I}\hat{D} = \hat{D}\hat{I}$

$\beta = 1$

$\beta = \begin{pmatrix} 0 & 1 & 0 \\ 1 & 0 & 0 \\ 0 & 0 & 1 \end{pmatrix}$

$\hat{A} = \hat{B} = \hat{C} = \hat{D} = \hat{I} = \hat{E}$
 $\hat{B}\hat{A} = \hat{A}\hat{B}; \hat{C}\hat{A} = \hat{B}\hat{C}$
 $\hat{C}\hat{B} = \hat{A}\hat{B}\hat{C}; \hat{D}\hat{A} = \hat{B}\hat{D}$
 $\hat{D}\hat{B} = \hat{B}\hat{D}; \hat{D}\hat{C} = \hat{C}\hat{D}$
 $\hat{I}\hat{A} = \hat{A}\hat{I}; \hat{I}\hat{B} = \hat{B}\hat{I}$
 $\hat{I}\hat{C} = \hat{C}\hat{I}; \hat{I}\hat{D} = \hat{D}\hat{I}$

$\beta = 1$

$\hat{A} = C_{2x}$
 $\hat{B} = C_{2y}$
 $\hat{C} = C_3$
 $\hat{D} = \theta C_2$
 $\hat{I} = S_2$

$\epsilon = \exp(2\pi i/3) = \frac{1}{2}(-1 + i\sqrt{3})$

I_h/I	E	$12C_5$	$12C_5^2$	$20C_3$	$15C_2$	θS_2	$12\theta S_{10}^3$	$12\theta S_{10}$	$12\theta S_6$	$15\theta\sigma$	$\tilde{A}^2 = \tilde{B}^2 = \tilde{C}^3 = \tilde{F}^5 = \tilde{I}^2 = \tilde{E}$ $\alpha_0 = 1$ $\tilde{B}\tilde{A} = \tilde{A}\tilde{B}; \tilde{C}\tilde{A} = \tilde{B}\tilde{C}; \tilde{C}\tilde{B} = \tilde{A}\tilde{B}\tilde{C}$ $\beta = 1$ $\tilde{F}\tilde{A} = \tilde{A}\tilde{F}^4; \tilde{F}\tilde{B} = \tilde{B}\tilde{C}^2\tilde{F}^2$ $\tilde{F}\tilde{C} = \tilde{C}^2\tilde{F}^4; \tilde{I}\tilde{A} = \tilde{A}\tilde{I}$ $\tilde{I}\tilde{B} = \tilde{B}\tilde{I}; \tilde{I}\tilde{C} = \tilde{C}\tilde{I}; \tilde{I}\tilde{F} = \tilde{F}\tilde{I}$
$D(A)$	1	1	1	1	1	1	1	1	1	1	
$\overline{D(A)}$	1	1	1	1	1	-1	-1	-1	-1	-1	
$D(T_1)$	3	Φ	$-\Phi^{-1}$	0	-1	3	Φ	$-\Phi^{-1}$	0	-1	
$D(T_2)$	3	$-\Phi^{-1}$	Φ	0	-1	3	$-\Phi^{-1}$	Φ	0	-1	
$\overline{D(T_1)}$	3	Φ	$-\Phi^{-1}$	0	-1	-3	$-\Phi$	Φ^{-1}	0	1	
$\overline{D(T_2)}$	3	$-\Phi^{-1}$	Φ	0	-1	-3	Φ^{-1}	$-\Phi$	0	1	
$D(G)$	4	-1	-1	1	0	4	-1	-1	1	0	
$\overline{D(G)}$	4	-1	-1	1	0	-4	1	1	-1	0	
$D(H)$	5	0	0	-1	1	5	0	0	-1	1	
$\overline{D(H)}$	5	0	0	-1	1	-5	0	0	1	-1	
I_h/I											$\tilde{A} = C_2$ $\tilde{B} = C_2$ $\tilde{C} = C_3$ $\tilde{F} = C_5$ $\tilde{I} = \theta S_2$

$$\Phi = \frac{1}{2}(\sqrt{5}+1) ; \Phi^{-1} = \frac{1}{2}(\sqrt{5}-1)$$

S'_{4n-2} / C'_{2n-1} $C'_{(2n-1)h} / C'_{2n-1}$ C'_{4n-2} / C'_{2n-1}	$1 \leq p \leq 2n-1$ A^{4n-2-p} A^p	$0 \leq q \leq 2n-2$ $A^{2q} B$	$0 \leq q \leq 2n-2$ $A^{2q+1} B$	$\tilde{A}^{4n-2} \tilde{B} = \tilde{E}$ $\tilde{B} \tilde{A} = \tilde{A}^{4n-3} \tilde{B}$	$a_6 = B$ $\beta = 1$
$D(B_{\frac{2n-1}{2}})$	1 $(-1)^p$	1	1		
$\overline{D(B_{\frac{2n-1}{2}})}$	1 $(-1)^p$	-1	-1		
$1 \leq l \leq n-1; D(E_{\frac{2l-1}{2}})$	2	$2 \cos(2l-1) p \pi / 2n-1$	0	0	

$\tilde{A} = C_{2n-1}; \tilde{B} = \theta C_2$
 $\tilde{A} = C_{2n-1} h; \tilde{B} = \theta \sigma h$
 $\tilde{A} = C_{2n-1}; \tilde{B} = \theta S_2$
 $n=1; \tilde{A}=R$

<p>n even ; C'_{2nh} / S'_{2n} n odd ; C'_{2nh} / C'_{nh} C'_{2nh} / C'_{2n}</p>	<p>$1 \leq p \leq 2n$ A^{4n-p} A^p</p>	<p>$0 \leq q \leq 2n-1$ $A^{2q} B$</p>	<p>$0 \leq q \leq 2n-1$ $A^{2q+1} B$</p>	<p>$\tilde{A}^{4n} \tilde{B}^{2n} = \tilde{E}$ $\tilde{B} \tilde{A} = \tilde{A}^{4n-1} \tilde{B}$ $a_0 = B$ $\beta = 1$</p>
<p>$1 \leq l \leq n ; D(E_{\frac{2n-1}{2}})$</p>	<p>2</p>	<p>$2 \cos(2l-1)\pi / 2n$</p>	<p>0</p>	<p>0</p>
<p>n odd ; C'_{2nh} / C'_{2n} n even ; C'_{2nh} / S'_{2n}</p>				<p>$\tilde{A} = C_{2n} ; \tilde{B} = \theta S_2$ $\tilde{A} = S_n^{2n-1} ; \tilde{B} = \theta S_2$ $\tilde{A} = S_{2n}^{2n-1} ; \tilde{B} = \theta S_2$</p>

$C'_{(4n-2)h}/S'_{4n-2}$	$1 \leq p \leq 2n-1$ A^{4n-2-p} A^p E	$0 \leq q \leq 2n-2$ $A^{2q}B$ $A^{2q+1}B$ $A^{2q}C$ $A^{2q+1}C$ $A^p C$	$0 \leq q \leq 2n-2$ $A^{2q}BC$ $A^{2q+1}BC$	$\tilde{A}^{4n-2} = \tilde{B}^2 \tilde{C}^2 = \tilde{E} \quad a_0 = B$ $\tilde{B}\tilde{A} = \tilde{A}^{4n-3} \tilde{B} \quad \beta = 1$ $\tilde{C}\tilde{A} = \tilde{A}\tilde{C}; \tilde{C}\tilde{B} = \tilde{B}\tilde{C}$	
$D(B_{\frac{2n-1}{2}}^g)$	1	1	1	-1	
$D(B_{\frac{2n-1}{2}}^u)$	1	1	$(-1)^p$	-1	1
$\overline{D(B_{\frac{2n-1}{2}}^g)}$	1	1	$(-1)^{p+1}$	-1	1
$\overline{D(B_{\frac{2n-1}{2}}^u)}$	1	-1	$(-1)^p$	-1	-1
$1 \leq l \leq n-1; D(E_{\frac{2l-1}{2}})$	2	$2 \cos(2l-1)p\pi/2n+1$	0	$2 \cos(2l-1)p\pi/2n+1$	0
$1 \leq l \leq n-1; \overline{D(E_{\frac{2l-1}{2}})}$	2	$2 \cos(2l-1)p\pi/2n+1$	0	$-2 \cos(2l-1)p\pi/2n+1$	0
$C'_{(4n-2)h}/S'_{4n-2}$					$\tilde{A} = C_{2n-1}; \tilde{A} = R \quad n=1$ $\tilde{B} = \theta C_2$ $\tilde{C} = S_2$

n even; D'_{nd} / S'_{2n} n odd; D'_{nh} / C'_{nh} D'_{2n} / C'_{2n} C'_{2nv} / C'_{2n}	$1 \leq p \leq 4n-1$ $E \quad A^p$	$0 \leq p \leq 4n$ $A^p B$	$\tilde{A} = \tilde{B} = \tilde{E}$ $\tilde{B} = \tilde{A} = \tilde{B}$ $\alpha_0 = B$ $\beta = 1$
$1 \leq l \leq n; D(E_{(2l-1)}^+)$ $D(E_{(2l-1)}^-)$	$1 \quad \exp i(2l-1)p\pi/2n$ $1 \quad \exp (-i(2l-1)p\pi)/2n$	$\exp i(2l-1)p\pi/2n$ $\exp (-i(2l-1)p\pi)/2n$	
$1 \leq l \leq n; \overline{D(E_{(2l-1)}^+)}$ $\overline{D(E_{(2l-1)}^-)}$	$1 \quad \exp i(2l-1)p\pi/2n$ $1 \quad \exp (-i(2l-1)p\pi)/2n$	$-\exp i(2l-1)p\pi/2n$ $-\exp (-i(2l-1)p\pi)/2n$	
C'_{2nv} / C'_{2n} D'_{2n} / C'_{2n} n odd; D'_{nh} / C'_{nh} n even; D'_{nd} / S'_{2n}			$\tilde{A} = C_{2n}; \tilde{B} = \theta \sigma_D$ $\tilde{A} = C_{2n}; \tilde{B} = \theta C'_2$ $\tilde{A} = S_n^{2n-1}; \tilde{B} = \theta C'_2$ $\tilde{A} = S_{2n}^{2n-1}; \tilde{B} = \theta \sigma_D$

n even; D'_{2nh} / D'_{nd} D'_{2nh} / D'_{nh} D'_{2nh} / D'_{2n} D'_{2nh} / C'_{2nv}	$1 \leq p \leq 2n$ A^{4n-p} E	$0 \leq p \leq 2n$ $A^{4n-p}C$ $A^{2q}B$	$0 \leq q \leq 2n-1$ $A^{2q+1}B$ $A^{2q}BC$ $A^{2q+1}BC$	$\tilde{A}^{4n} \tilde{B}^4 \tilde{C}^2 \tilde{E}$ $\tilde{A}^{2n} \tilde{B}^2$ $\tilde{B} \tilde{A} = \tilde{A}^{4n-1} \tilde{B}$ $\tilde{C} \tilde{A} = \tilde{A} \tilde{C}; \tilde{C} \tilde{B} = \tilde{B} \tilde{C}$	$\alpha_2 R$ $\beta = \begin{pmatrix} 0 & 1 \\ -1 & 0 \end{pmatrix}$
$1 \leq l \leq n; D(E_{\frac{(2l-1)}{2}})$	2 $2 \cos(2l-1)p\pi/2n$ 0	0	0 0	0	
$1 \leq l \leq n; \overline{D}(E_{\frac{(2l-1)}{2}})$	2 $2 \cos(2l-1)p\pi/2n$ 0	0	0 $-2 \cos(2l-1)p\pi/2n$	0	
n even; D'_{2nh} / C'_{2nv} D'_{2nh} / D'_{2n} D'_{2nh} / D'_{nh} D'_{2nh} / D'_{nd}					$\tilde{A} = C_{2n}; \tilde{B} = \sigma_v; \tilde{C} = \theta S_2$ $\tilde{A} = C_{2n}; \tilde{B} = C'_2; \tilde{C} = \theta S_2$ $\left\{ \begin{array}{l} n \text{ odd } \tilde{A} = S_{2n}^{2n-1}; \tilde{B} = C'_2; \tilde{C} = \theta S_2 \\ n \text{ even } \tilde{A} = C_{2n}; \tilde{B} = \sigma_v; \tilde{C} = \theta C'_2 \\ \tilde{A} = S_{2n}^{2n+1}; \tilde{B} = C'_2; \tilde{C} = \theta S_2 \end{array} \right.$

D'_{2nh} / C'_{2nh}	$E \quad A^p$	$0 \leq p \leq 4n$	$0 \leq p \leq 4n-1$	$0 \leq p \leq 4n$	$A^p B$	$A^p C$	$A^p BC$	$0 \leq p \leq 4n$	$\tilde{A} = B = \tilde{C} = E$ $\tilde{B} = \tilde{A} = \tilde{C} = E$ $\tilde{C} = \tilde{A} = \tilde{B} = \tilde{C} = E$	$\alpha_0 = R$ $\beta = 1$
$1 \leq l \leq n; D(E_{(\frac{2l-1}{2})})$ $\left\{ \begin{array}{l} D(E_{(\frac{2l-1}{2})}^+) \\ D(E_{(\frac{2l-1}{2})}^-) \end{array} \right.$		$\exp i(2l-1)p\pi/2n$	$\exp i(2l-1)p\pi/2n$	$\exp i(2l-1)p\pi/2n$	$\exp i(2l-1)p\pi/2n$	$\exp i(2l-1)p\pi/2n$	$\exp i(2l-1)p\pi/2n$	$\exp i(2l-1)p\pi/2n$		
		$\exp(-i(2l-1)p\pi)/2n$	$\exp(-i(2l-1)p\pi)/2n$	$\exp(-i(2l-1)p\pi)/2n$	$\exp(-i(2l-1)p\pi)/2n$	$\exp(-i(2l-1)p\pi)/2n$	$\exp(-i(2l-1)p\pi)/2n$	$\exp(-i(2l-1)p\pi)/2n$		
		$\exp i(2l-1)p\pi/2n$	$-\exp i(2l-1)p\pi/2n$	$\exp i(2l-1)p\pi/2n$	$-\exp i(2l-1)p\pi/2n$	$\exp i(2l-1)p\pi/2n$	$-\exp i(2l-1)p\pi/2n$	$-\exp i(2l-1)p\pi/2n$		
		$\exp(-i(2l-1)p\pi)/2n$	$-\exp(-i(2l-1)p\pi)/2n$	$\exp(-i(2l-1)p\pi)/2n$	$-\exp(-i(2l-1)p\pi)/2n$	$\exp(-i(2l-1)p\pi)/2n$	$-\exp(-i(2l-1)p\pi)/2n$	$-\exp(-i(2l-1)p\pi)/2n$		
$1 \leq l \leq n; D(E_{(\frac{2l}{2})})$ $\left\{ \begin{array}{l} D(E_{(\frac{2l}{2})}^+) \\ D(E_{(\frac{2l}{2})}^-) \end{array} \right.$		$\exp i(2l-1)p\pi/2n$	$\exp i(2l-1)p\pi/2n$	$-\exp i(2l-1)p\pi/2n$	$-\exp i(2l-1)p\pi/2n$	$\exp i(2l-1)p\pi/2n$	$-\exp i(2l-1)p\pi/2n$	$-\exp i(2l-1)p\pi/2n$		
		$\exp(-i(2l-1)p\pi)/2n$	$\exp(-i(2l-1)p\pi)/2n$	$-\exp(-i(2l-1)p\pi)/2n$	$-\exp(-i(2l-1)p\pi)/2n$	$\exp(-i(2l-1)p\pi)/2n$	$-\exp(-i(2l-1)p\pi)/2n$	$\exp(-i(2l-1)p\pi)/2n$		
		$\exp i(2l-1)p\pi/2n$	$-\exp i(2l-1)p\pi/2n$	$\exp i(2l-1)p\pi/2n$	$-\exp i(2l-1)p\pi/2n$	$-\exp i(2l-1)p\pi/2n$	$-\exp i(2l-1)p\pi/2n$	$-\exp i(2l-1)p\pi/2n$		
		$\exp(-i(2l-1)p\pi)/2n$	$-\exp(-i(2l-1)p\pi)/2n$	$\exp(-i(2l-1)p\pi)/2n$	$-\exp(-i(2l-1)p\pi)/2n$	$\exp(-i(2l-1)p\pi)/2n$	$-\exp(-i(2l-1)p\pi)/2n$	$\exp(-i(2l-1)p\pi)/2n$		
$1 \leq l \leq n; \overline{D(E_{(\frac{2l-1}{2})})}$ $\left\{ \begin{array}{l} \overline{D(E_{(\frac{2l-1}{2})}^+)}$ $\overline{D(E_{(\frac{2l-1}{2})}^-)}$		$\exp i(2l-1)p\pi/2n$	$\exp i(2l-1)p\pi/2n$	$-\exp i(2l-1)p\pi/2n$	$-\exp i(2l-1)p\pi/2n$	$\exp i(2l-1)p\pi/2n$	$-\exp i(2l-1)p\pi/2n$	$-\exp i(2l-1)p\pi/2n$		
		$\exp(-i(2l-1)p\pi)/2n$	$\exp(-i(2l-1)p\pi)/2n$	$-\exp(-i(2l-1)p\pi)/2n$	$-\exp(-i(2l-1)p\pi)/2n$	$\exp(-i(2l-1)p\pi)/2n$	$-\exp(-i(2l-1)p\pi)/2n$	$\exp(-i(2l-1)p\pi)/2n$		
		$\exp i(2l-1)p\pi/2n$	$-\exp i(2l-1)p\pi/2n$	$\exp i(2l-1)p\pi/2n$	$-\exp i(2l-1)p\pi/2n$	$-\exp i(2l-1)p\pi/2n$	$-\exp i(2l-1)p\pi/2n$	$-\exp i(2l-1)p\pi/2n$		
		$\exp(-i(2l-1)p\pi)/2n$	$-\exp(-i(2l-1)p\pi)/2n$	$\exp(-i(2l-1)p\pi)/2n$	$-\exp(-i(2l-1)p\pi)/2n$	$\exp(-i(2l-1)p\pi)/2n$	$-\exp(-i(2l-1)p\pi)/2n$	$\exp(-i(2l-1)p\pi)/2n$		
D'_{2nh} / C'_{2nh}										$\tilde{A} = C_{2n}$ $\tilde{B} = S_2$ $\tilde{C} = \theta C_2$

C'_{4n}/C'_{2n}	E $1 \leq p \leq 2n$ A^{8n-2p} P^{2p}	$0 \leq q \leq 2n-1$ A^{4q+1} $0 \leq q \leq 2n-1$ A^{4q+3}	$\tilde{A}^{4n} = \tilde{B}^{4n} = \tilde{E}$ $\tilde{B}^2 = \tilde{A}^{2n}$ $\tilde{B}\tilde{A} = \tilde{A}^{4n-1}\tilde{B}$	$\alpha_0 = \beta$ $\beta = 1$
$1 \leq k \leq n; D(E^{(\frac{2k-1}{2})})$	2 $2 \cos(2k-1)\pi/2n$	0 0		
C'_{4n}/C'_{2n}			$\tilde{A} = C_{2n}$ $\tilde{B} = \theta C_{4n}$	

D'_{2nd}/D'_{2n} D'_{4n}/D'_{2n} D'_{2nd}/C'_{2nv} C'_{4nv}/C'_{2nv}	$1 \leq p \leq 4n$ A^{8n-p} A^p	$0 \leq q \leq 4n-1$ $A^{2q+1} B$	$\tilde{A}^p = \tilde{B}^4 = E$ $\tilde{B}^2 = \tilde{A}^{4n}$ $\tilde{B} \tilde{A} = \tilde{A}^{8n-1} \tilde{B}$	$\alpha_0 = P$
$1 \leq l \leq n; D(E_{\frac{2l-1}{2}})$	$2 \quad 2 \cos(2l-1)p\pi/4n$	$0 \quad 0$	$\beta = \begin{pmatrix} e^{-i\sqrt{2}en} & 0 \\ 0 & e^{i\sqrt{2}en} \end{pmatrix}$	
$1 \leq l \leq n; D(E_{\frac{2l+1}{2}})$	$2 \quad (-1)^p 2 \cos(2l-1)p\pi/4n$	$0 \quad 0$		
C'_{4nv}/C'_{2nv} D'_{2nd}/C'_{2nv} D'_{4n}/D'_{2n} D'_{2nd}/D'_{2n}				$\tilde{A} = \theta \sigma_3; \tilde{B} = \sigma_4$ $\tilde{A} = \theta C'_2; \tilde{B} = \sigma_4$ $\tilde{A} = \theta C'_2; \tilde{B} = C_2$ $\tilde{A} = \theta \sigma_3; \tilde{B} = C_2$

C_{4nh} / C_{2nh}	E	$1 \leq p \leq 2n$ A^{2p} A^{4p+1}	$0 \leq q \leq 2n-1$ A^{2p} A^{4q+3}	$0 \leq p \leq 2n$ A^{2n-2p} A^{2p}	$0 \leq q \leq 2n-1$ A^{4q+1} A^{4q+3}	$0 \leq q \leq 2n-1$ A^{4q+1} A^{4q+3}	$\tilde{A} = \tilde{B} = \tilde{C} = \tilde{E}$ $\tilde{B} = \tilde{A}^{2n}$ $\tilde{C} = \tilde{A}^{4n-1}$	$\alpha_0 = B$ $\beta = 1$ $\tilde{C} = \tilde{B} = \tilde{C}$ $\tilde{C} = \tilde{A} = \tilde{C}$
$1 \leq l \leq n; D(E_{(2,2-1)q})$	2	$2 \cos(2l-1)\pi/2n$	0	0	$2 \cos(2l-1)\pi/2n$	0		
$1 \leq l \leq n; D(E_{(2,2-1)q})$	2	$2 \cos(2l-1)\pi/2n$	0	0	$-2 \cos(2l-1)\pi/2n$	0		
C'_{4nh} / C'_{2nh}							$\tilde{A} = C_{2n}$ $\tilde{B} = \theta C_{4n}$ $\tilde{C} = S_2$	

$\frac{D'_{2n+1}}{C'_{2n+1}} / \frac{C'_{2n+1}}{C'_{2n+1}}$	$1 \leq p \leq 4n-3$ $E \quad A^p$	$0 \leq p \leq 4n-3$ $A^p B$	$\tilde{A}^{4n+2} \tilde{B}^2 = \tilde{E}$ $\tilde{B} \tilde{A} = \tilde{A} \tilde{B}$	$\alpha_0 = B$ $\beta = 1$
$D(B_{\frac{2n+1}{2}})$	$1 \quad (-1)^p$	$(-1)^p$		
$\overline{D(B_{\frac{2n+1}{2}})}$	$1 \quad (-1)^p$	$(-1)^{p+1}$		
$\left. \begin{matrix} D(E_{\frac{(2l-1)}{2}}^+) \\ D(E_{\frac{(2l-1)}{2}}^-) \end{matrix} \right\} 1 \leq l \leq n$	$1 \quad \exp(i(2l-1)p\pi/2n+1)$	$\exp(i(2l-1)p\pi/2n+1)$		
$\left. \begin{matrix} \overline{D(E_{\frac{(2l-1)}{2}}^+)} \\ \overline{D(E_{\frac{(2l-1)}{2}}^-)} \end{matrix} \right\} 1 \leq l \leq n$	$1 \quad \exp(i(2l-1)p\pi/2n+1)$	$\exp(i(2l-1)p\pi/2n+1)$		
$\left. \begin{matrix} D(E_{\frac{(2l-1)}{2}}^+) \\ D(E_{\frac{(2l-1)}{2}}^-) \end{matrix} \right\} 1 \leq l \leq n$	$1 \quad \exp(i(2l-1)p\pi/2n+1)$	$-\exp(i(2l-1)p\pi/2n+1)$		
$\left. \begin{matrix} \overline{D(E_{\frac{(2l-1)}{2}}^+)} \\ \overline{D(E_{\frac{(2l-1)}{2}}^-)} \end{matrix} \right\} 1 \leq l \leq n$	$1 \quad \exp(i(2l-1)p\pi/2n+1)$	$-\exp(i(2l-1)p\pi/2n+1)$		
$\frac{C'_{2n+1}}{C'_{2n+1}} / \frac{C'_{2n+1}}{C'_{2n+1}}$			$\tilde{A} = C_{2n+1}; B = \theta \sigma \tilde{B}$ $\tilde{A} = C_{2n+1}; B = \theta C'_2$	

$D'_{(4n+2)}/D'_{(2n+1)}$ $D'_{(2n+1)h}/D'_{(2n+1)}$ $D'_{(2n+1)h}/C'_{(2n+1)h}$ $C'_{(4n+2)h}/C'_{(2n+1)h}$	E $1 \leq p \leq 2n+1$ A^{4n+2-p} A^p	$0 \leq q \leq 2n$ $A^{2q}B$	$0 \leq p \leq 2n+1$ $A^{4n+2-p}C$ A^pC	$0 \leq q \leq 2n$ $A^{2q}BC$	$\tilde{A}^{4n+2} \tilde{B} \tilde{C} \tilde{E}$ $\alpha_0 = R$ $\tilde{A}^{2n+1} \tilde{B}^2$ $\beta = 1$ $\tilde{B} \tilde{A} = \tilde{A}^{4n+1} \tilde{B}$ $\tilde{C} \tilde{A} = \tilde{A} \tilde{C}; \tilde{C} \tilde{B} = \tilde{B} \tilde{C}$
$D(E_{\frac{2n+1}{2}})$	$(-1)^p$	i	$(-1)^p$	i	$-i$
$D(E_{\frac{2n+1}{2}})$	$(-1)^p$	$-i$	$(-1)^p$	$-i$	i
$D(E_{\frac{2n+1}{2}})$	$(-1)^p$	i	$(-1)^{p+1}$	$-i$	i
$D(E_{\frac{2n+1}{2}})$	$(-1)^p$	$-i$	$(-1)^{p+1}$	i	$-i$
$1 \leq l \leq n$ $D(E_{\frac{2l-1}{2}})$	$2 \cos(2l-1)p\pi/2n+1$	0	$2 \cos(2l-1)p\pi/2n+1$	0	0
$1 \leq l \leq n$ $D(E_{\frac{2l-1}{2}})$	$2 \cos(2l-1)p\pi/2n+1$	0	$-2 \cos(2l-1)p\pi/2n+1$	0	0
$C'_{(4n+2)h}/C'_{(2n+1)h}$ $D'_{(2n+1)h}/C'_{(2n+1)h}$ $D'_{(2n+1)h}/D'_{(2n+1)}$ $D'_{(4n+2)}/D'_{(2n+1)}$	$\tilde{A} = C_{2n+1}; \tilde{B} = \sigma; \tilde{C} = \theta C_2$ $\tilde{A} = C_{2n+1}; \tilde{B} = \sigma; \tilde{C} = \theta \sigma_1$ $\tilde{A} = C_{2n+1}; \tilde{B} = C_2; \tilde{C} = \theta \sigma_1$ $\tilde{A} = C_{2n+1}; \tilde{B} = C_2; \tilde{C} = \theta C_2$				

$D'_{(2n+1)l} / S'_{4n+2}$	$1 \leq p \leq 4n+1$	$0 \leq p \leq 4n+1$	$0 \leq p \leq 4n+1$	$0 \leq p \leq 4n+1$	$\tilde{A} = S_{4n+2}$ $\tilde{B} = S_2$ $\tilde{C} = \theta C_2$
E AP	APB	APC	APBC		
$D \left(B_{\frac{(2n+1)g}{2}} \right)$	$(-1)^p$	$(-1)^p$	$(-1)^p$	$(-1)^p$	
$D \left(B_{\frac{(2n+1)u}{2}} \right)$	$(-1)^{p+1}$	$(-1)^{p+1}$	$(-1)^{p+1}$	$(-1)^{p+1}$	
$D \left(B_{\frac{(2n+1)g}{2}} \right)$	$(-1)^p$	$(-1)^p$	$(-1)^p$	$(-1)^p$	
$D \left(B_{\frac{(2n+1)u}{2}} \right)$	$(-1)^{p+1}$	$(-1)^{p+1}$	$(-1)^{p+1}$	$(-1)^{p+1}$	
$\left. \begin{matrix} D \left(E_{(2l-1)g} \right) \\ D \left(E_{(2l-1)u} \right) \end{matrix} \right\}$	$\exp(i(2l-1)p\pi/2n+1)$	$\exp(i(2l-1)p\pi/2n+1)$	$\exp(i(2l-1)p\pi/2n+1)$	$\exp(i(2l-1)p\pi/2n+1)$	
$\left. \begin{matrix} D \left(E_{(2l-1)g} \right) \\ D \left(E_{(2l-1)u} \right) \end{matrix} \right\}$	$\exp(-i(2l-1)p\pi/2n+1)$	$\exp(-i(2l-1)p\pi/2n+1)$	$\exp(-i(2l-1)p\pi/2n+1)$	$\exp(-i(2l-1)p\pi/2n+1)$	
$\left. \begin{matrix} D \left(E_{(2l-1)g} \right) \\ D \left(E_{(2l-1)u} \right) \end{matrix} \right\}$	$\exp(i(2l-1)p\pi/2n+1)$	$\exp(i(2l-1)p\pi/2n+1)$	$\exp(i(2l-1)p\pi/2n+1)$	$\exp(i(2l-1)p\pi/2n+1)$	
$\left. \begin{matrix} D \left(E_{(2l-1)g} \right) \\ D \left(E_{(2l-1)u} \right) \end{matrix} \right\}$	$\exp(-i(2l-1)p\pi/2n+1)$	$\exp(-i(2l-1)p\pi/2n+1)$	$\exp(-i(2l-1)p\pi/2n+1)$	$\exp(-i(2l-1)p\pi/2n+1)$	
$\left. \begin{matrix} D \left(E_{(2l-1)g} \right) \\ D \left(E_{(2l-1)u} \right) \end{matrix} \right\}$	$\exp(i(2l-1)p\pi/2n+1)$	$\exp(i(2l-1)p\pi/2n+1)$	$\exp(i(2l-1)p\pi/2n+1)$	$\exp(i(2l-1)p\pi/2n+1)$	
$\left. \begin{matrix} D \left(E_{(2l-1)g} \right) \\ D \left(E_{(2l-1)u} \right) \end{matrix} \right\}$	$\exp(-i(2l-1)p\pi/2n+1)$	$\exp(-i(2l-1)p\pi/2n+1)$	$\exp(-i(2l-1)p\pi/2n+1)$	$\exp(-i(2l-1)p\pi/2n+1)$	
$D'_{(2n+1)l} / S_{4n+2}$					

$$\tilde{A}_{4n+2} = \tilde{C}_2 = \tilde{E}$$

$$\tilde{B} = \tilde{A}\tilde{B}; \tilde{C}\tilde{A} = \tilde{A}\tilde{C}$$

$$\tilde{C}\tilde{B} = \tilde{B}\tilde{C}$$

$$a_0 = R$$

$$\beta = 1$$

$$\tilde{A} = S_{4n+2}$$

$$\tilde{B} = S_2$$

$$\tilde{C} = \theta C_2$$

	$1 \leq p \leq 4n+2$ A^{8n-4-p} P^p	$0 \leq q \leq 4n+1$ $A^{2q} B$ $A^{2q+1} B$	$\tilde{A}^{8n+4} = \tilde{B}^4 = E$ $\tilde{A}^{4n+2} = \tilde{B}^2$ $\tilde{B} \tilde{A} = \rho^{8n+3} B$	$\alpha_p = \rho^{2n+1}$
$D'_{(2n+1)d} / D'_{2n+1}$ $D'_{(2n+1)d} / C'_{(2n+1)v}$	E			
$D(E_{\frac{2n+1}{2}})$	2	$2 \cos p\pi/2$	0 0	0
$1 \leq l \leq n; D(E_{\frac{2l-1}{2}})$	2	$2 \cos(2l-1)p\pi/4n+2$	0 0	0
$1 \leq l \leq n; D(E_{\frac{2l-1}{2}})$	2	$(-1)^p 2 \cos(2l-1)p\pi/4n+2$	0 0	0
$D'_{(2n+1)d} / C'_{(2n+1)v}$ $D'_{(2n+1)d} / D'_{2n+1}$			$\tilde{A} = \theta S_{4n+2}; \tilde{B} = \sigma v$ $\tilde{A} = \theta S_{4n+2}; \tilde{B} = C'_2$	$\beta = \begin{pmatrix} 0 & 1 \\ -1 & 0 \end{pmatrix}$

$D'_{(4n+2)h} / D'_{(2n+1)}$	$1 \leq p \leq 2n+1$	$0 \leq q \leq 2n$	$0 \leq p \leq 2n+1$	$0 \leq q \leq 2n$	$0 \leq p \leq 2n+1$	$0 \leq q \leq 2n$	$0 \leq q \leq 2n$	$0 \leq q \leq 2n$	$0 \leq q \leq 2n$
	A^{4n+2-p}	$A^{2q} B A^{2q+1} B$	$A^{4n+2-p} C$	$A^{2q} B C A^{2q+1} B$	$A^{4n+2-p} D$	$A^{2q} B D A^{2q+1} B D$	$A^{2q} B C D$	$A^{2q+1} B C D$	$A^{4n+2-p} C D$
	$E A^p$	$A^{2q} B A^{2q+1} B$	$A^{4n+2-p} C$	$A^{2q} B C A^{2q+1} B$	$A^{4n+2-p} D$	$A^{2q} B D A^{2q+1} B D$	$A^{2q} B C D$	$A^{2q+1} B C D$	$A^{4n+2-p} C D$
$D(E^{(\frac{2n+1}{2})g})$	$(-1)^p$	i	$(-1)^p$	i	$(-1)^p$	i	i	i	$(-1)^p$
$D(E^{(\frac{2n+1}{2})g})$	$(-1)^p$	$-i$	$(-1)^p$	$-i$	$(-1)^p$	$-i$	$-i$	$-i$	$(-1)^p$
$D(E^{(\frac{2n+1}{2})u})$	$(-1)^p$	i	$(-1)^{p+1}$	i	$(-1)^p$	i	i	i	$(-1)^{p+1}$
$D(E^{(\frac{2n+1}{2})u})$	$(-1)^p$	$-i$	$(-1)^{p+1}$	$-i$	$(-1)^p$	$-i$	$-i$	$-i$	$(-1)^{p+1}$
$D(E^{(\frac{2n+1}{2})g})$	$(-1)^p$	i	$(-1)^p$	i	$(-1)^{p+1}$	i	i	i	$(-1)^{p+1}$
$D(E^{(\frac{2n+1}{2})g})$	$(-1)^p$	$-i$	$(-1)^{p+1}$	$-i$	$(-1)^{p+1}$	$-i$	$-i$	$-i$	$(-1)^{p+1}$
$D(E^{(\frac{2n+1}{2})u})$	$(-1)^p$	i	$(-1)^{p+1}$	i	$(-1)^{p+1}$	i	i	i	$(-1)^{p+1}$
$D(E^{(\frac{2n+1}{2})u})$	$(-1)^p$	$-i$	$(-1)^{p+1}$	$-i$	$(-1)^{p+1}$	$-i$	$-i$	$-i$	$(-1)^{p+1}$
$1 \leq l \leq n$; $D(E^{(\frac{2l-1}{2})g})$	$2 \cos(2l-1)p\pi/2n+1$	0	$2 \cos(2l-1)p\pi/2n+1$	0	$2 \cos(2l-1)p\pi/2n+1$	0	0	0	$2 \cos(2l-1)p\pi/2n+1$
$1 \leq l \leq n$; $D(E^{(\frac{2l-1}{2})u})$	$2 \cos(2l-1)p\pi/2n+1$	0	$-2 \cos(2l-1)p\pi/2n+1$	0	$2 \cos(2l-1)p\pi/2n+1$	0	0	0	$-2 \cos(2l-1)p\pi/2n+1$
$1 \leq l \leq n$; $D(E^{(\frac{2l-1}{2})g})$	$2 \cos(2l-1)p\pi/2n+1$	0	$2 \cos(2l-1)p\pi/2n+1$	0	$-2 \cos(2l-1)p\pi/2n+1$	0	0	0	$-2 \cos(2l-1)p\pi/2n+1$
$1 \leq l \leq n$; $D(E^{(\frac{2l-1}{2})u})$	$2 \cos(2l-1)p\pi/2n+1$	0	$-2 \cos(2l-1)p\pi/2n+1$	0	$-2 \cos(2l-1)p\pi/2n+1$	0	0	0	$2 \cos(2l-1)p\pi/2n+1$
$D_{(4n+2)h} / D_{(2n+1)}$									

$$\tilde{A} = \tilde{A}^{4n+2} \tilde{B} = \tilde{C} = \tilde{D} = \tilde{E}$$

$$\tilde{A} = \tilde{B}$$

$$\tilde{B} \tilde{A} = \tilde{A}^{4n+1} \tilde{B}; \tilde{D} \tilde{C} = \tilde{C} \tilde{D}$$

$$\tilde{C} \tilde{A} = \tilde{A} \tilde{C}; \tilde{C} \tilde{B} = \tilde{B} \tilde{C}$$

$$\tilde{D} \tilde{A} = \tilde{A} \tilde{D}; \tilde{D} \tilde{B} = \tilde{B} \tilde{D}$$

$$\alpha_0 = D$$

$$\beta = 1$$

$$\tilde{A} = S_{2n-1}$$

$$\tilde{B} = C'_2$$

$$\tilde{C} = S_2$$

$$\tilde{D} = \theta C_2$$

T'_h/T'	E	P^3	Q, P^3Q	P, P^5	I	RI	P^3I	PI, P^2RI	P^2QI, P^4RI	P^5QI, P^3QRI	P^4QI, P^5QRI	P^5I, P^5RI	P^4I, PRI
$D(E_{\frac{1}{2}})$	2	-2	0	1	0	-2	2	1	-1				
$\overline{D}(E_{\frac{1}{2}})$	2	-2	0	1	0	2	-2	-1	1				
$D(G_{\frac{3}{2}})$	4	-4	0	-1	1	0	0	0	0	0			

$\alpha_0 = I$	$\beta = \begin{pmatrix} 0 & 1 \\ -1 & 0 \end{pmatrix}$
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$\tilde{P} = \tilde{Q} = \tilde{R} = \tilde{I} = \tilde{E}$; $\tilde{P}^2 = \tilde{Q}^2 = \tilde{R}^2$; $\tilde{I}\tilde{P} = \tilde{P}\tilde{I}$; $\tilde{I}\tilde{Q} = \tilde{Q}\tilde{I}$; $\tilde{Q}\tilde{P} = \tilde{P}\tilde{Q}$; $\tilde{R}\tilde{P} = \tilde{P}\tilde{Q}\tilde{R}$; $\tilde{R}\tilde{Q} = \tilde{P}^3\tilde{Q}\tilde{R}$; $\tilde{I}\tilde{R} = \tilde{R}\tilde{I}$
$\tilde{A}^4 = \tilde{B}^4 = \tilde{C} = \tilde{D} = \tilde{E}$; $\tilde{P}^2 = \tilde{Q}^2 = \tilde{D}^2$; $\tilde{D}\tilde{E} = \tilde{A}^3\tilde{D}$; $\tilde{B}\tilde{A} = \tilde{A}^3\tilde{B}$; $\tilde{C}\tilde{A} = \tilde{B}\tilde{C}$; $\tilde{C}\tilde{B} = \tilde{A}\tilde{B}\tilde{C}$; $\tilde{D}\tilde{A} = \tilde{A}^3\tilde{B}\tilde{D}$; $\tilde{D}\tilde{C} = \tilde{C}^2\tilde{D}$
$\tilde{P} = C_3$; $\tilde{Q} = C_{1x}$; $\tilde{R} = RC_{2y}$; $\tilde{I} = \theta S_2$ $\tilde{A} = C_{2x}$; $\tilde{B} = C_{2y}$; $\tilde{C} = RC_3$; $\tilde{D} = \theta C_2$

T_d/T'	ABC^2, A^2C	A^2C, A^2C^2	BC^2D, A^2BC^2D	A^2C^2D	A^2D	A^2B^4, C^3, D^3, E
O'/T'	AB, A^2B	BC, A^2BC	BCD, A^2BCD	A^2CD	A^2BD	A^2B^2, D^2
$D(E_{1/2})$	B, A^2B	AC, A^2BC	C^2D, A^2C^2D	ABC^2D	A^2D	$B\tilde{A} = \tilde{A}\tilde{B}; \tilde{C}\tilde{A} = \tilde{B}\tilde{C}$
$\overline{D(E_{1/2})}$	A, A^2	A^2C	BD, A^2D	ABD	A^2BCD	$\tilde{C}\tilde{B} = \tilde{A}\tilde{B}\tilde{C}$
O'/T'	E	C, C^2	AD, A^2BD	D	CD	$\tilde{D}\tilde{A} = \tilde{A}^2\tilde{B}\tilde{D}; \tilde{D}\tilde{B} = \tilde{A}^3\tilde{D}$
T_d/T'	$2 - 2$	$1 - 1$	0	$\sqrt{2}$	$-\sqrt{2}$	$\tilde{D}\tilde{C} = \tilde{C}^2\tilde{D}$
$\overline{D(E_{1/2})}$	$2 - 2$	$1 - 1$	0	$-\sqrt{2}$	$\sqrt{2}$	$\alpha_0 = D$
O'/T'						$\beta = \frac{1}{\sqrt{2}} \begin{pmatrix} 1+i & 0 \\ 0 & 1-i \end{pmatrix}$
T_d/T'						$\tilde{A} = C_{2x}; \tilde{B} = C_{2y}; \tilde{C} = RC_3; \tilde{D} = \theta C_2$
$\overline{D(E_{1/2})}$						$\tilde{A} = C_{2x}; \tilde{B} = C_{2y}; \tilde{C} = RC_3; \tilde{D} = \theta C_2$

T_d/T'	AC	A^2BC^2, AC^2, A^2BC	A^2BCD	A^2BCD	A^2BCD	A^2B^4, C^3, D^3, E
O'/T'	AB, A^2B	BC, A^2C^2, BC^2, A^2BC	A^2BD	A^2BCD	A^2BCD	A^2B^2, D^2
$D(G_{3/2})$	B, A^2B	$ABC, A^2BC^2, ABC^2, A^2C$	BD	A^2BCD	A^2BCD	$B\tilde{A} = \tilde{A}^3\tilde{B}; \tilde{C}\tilde{A} = \tilde{B}\tilde{C}$
$\overline{D(G_{3/2})}$	A, A^2	A^2C, A^2C^2, C, C^2	A^2D	ACD	A^2CD	$\tilde{C}\tilde{B} = \tilde{A}\tilde{B}\tilde{C}$
$D(G_{3/2})$	$2 - 2$	$\omega^* - \omega^*$	$2 - 2$	ω^*	$-\omega^*$	$\tilde{D}\tilde{A} = \tilde{A}^2\tilde{D}; \tilde{D}\tilde{B} = \tilde{B}\tilde{D}$
$\overline{D(G_{3/2})}$	$2 - 2$	$\omega - \omega$	$2 - 2$	ω	$-\omega$	$\tilde{D}\tilde{C} = \tilde{C}\tilde{D}$
O'/T'	$2 - 2$	$\omega^* - \omega^*$	$2 - 2$	ω^*	$-\omega^*$	$\alpha_0 = D$
T_d/T'	$2 - 2$	$\omega - \omega$	$2 - 2$	ω	$-\omega$	$\beta = \begin{pmatrix} 0 & -i \\ -i & 0 \end{pmatrix}$
$\overline{D(G_{3/2})}$	$2 - 2$	$\omega^* - \omega^*$	$2 - 2$	ω^*	$-\omega^*$	$\tilde{A} = C_{2x}; \tilde{B} = C_{2y}; \tilde{C} = RC_3; \tilde{D} = \theta C_2$
O'/T'						$\tilde{A} = C_{2x}; \tilde{B} = C_{2y}; \tilde{C} = RC_3; \tilde{D} = \theta C_2$
T_d/T'						$\tilde{A} = C_{2x}; \tilde{B} = C_{2y}; \tilde{C} = RC_3; \tilde{D} = \theta C_2$

$$\omega = \exp 2\pi i / 3 = -\frac{1}{2} + \frac{i\sqrt{3}}{2}$$

O_h/T_h		E	A_1	A_2	B_1	B_2	C	D	E	F	G	H	I	J	K	L	M	N	O	P	Q	R	S	T	U	V	W	X	Y	Z				
$D(E_{g1})$		2	-2	0	1	-1	0	$\sqrt{2}$	$-\sqrt{2}$	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0		
$D(E_{g2})$		2	-2	0	1	-1	0	$-\sqrt{2}$	$\sqrt{2}$	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	
$D(E_{g3})$		2	-2	0	1	-1	0	$\sqrt{2}$	$-\sqrt{2}$	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
$D(E_{g4})$		2	-2	0	1	-1	0	$-\sqrt{2}$	$\sqrt{2}$	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0

O_h/T_h		E	A_1	A_2	B_1	B_2	C	D	E	F	G	H	I	J	K	L	M	N	O	P	Q	R	S	T	U	V	W	X	Y	Z					
$D(G_{32g})$		2	-2	0	1	-1	0	$\sqrt{2}$	$-\sqrt{2}$	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	
$D(G_{32g})$		2	-2	0	1	-1	0	$-\sqrt{2}$	$\sqrt{2}$	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
$D(G_{32g})$		2	-2	0	1	-1	0	$\sqrt{2}$	$-\sqrt{2}$	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
$D(G_{32g})$		2	-2	0	1	-1	0	$-\sqrt{2}$	$\sqrt{2}$	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0

$$\omega = \exp\left(\frac{2\pi i}{3}\right) = -\frac{1}{2} + i\frac{\sqrt{3}}{2}$$

$A = G_{2g}; B = G_{2g}; C = RC_3;$
 $D = \theta C_2; E = S_2$

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