

Ray Representations of Point Groups and the Irreducible Representations of Space Groups and Double Space Groups

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RAY REPRESENTATIONS OF POINT GROUPS AND THE IRREDUCIBLE REPRESENTATIONS OF SPACE GROUPS AND DOUBLE SPACE GROUPS

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The theory of the ray representations of a finite group is summarized and full matrix ray representations are derived and tabulated for all thirty-two point groups. It is shown that any irreducible representation of any of the 230 space groups and of the corresponding double groups may be obtained quickly and easily from these ray representations of the point groups. The most complex cases which arise, namely points of high symmetry on the surface of the Brillouin zone for the regular holohedric space groups, $O_h^1 \dots O_h^{10}$, are treated explicitly. The relation of the present work to the recent treatments of Slater and Kovalev is discussed.

1. INTRODUCTION

For some applications of group theory to chemical and physical problems one needs explicit matrices for the various irreducible representations; the characters of the representations are not sufficient. For example, projection operators constructed from the full matrices can be used to resolve an arbitrary function into components, each of which transforms as a partner in a particular irreducible representation (McWeeny 1963; Slater 1963). This transformation is useful not only in general theoretical discussions but also in numerical calculations for specific systems since it simplifies the secular equations and other key relations.

Although the characters of the representations suffice for an analysis of degeneracies and selection rules, and of the way in which these change under various perturbations, they are not very helpful in simplifying numerical calculations. This is because the resolution of an

arbitrary function provided by a character projection operator may be so incomplete as to be almost useless. An extreme case occurs for certain representations of space groups which have non-zero characters only for the identity rotation. Clearly a projection operator constructed from such a character is valueless.

Explicit matrices are available for all irreducible representations of the thirty-two point groups (McWeeny 1963; Slater 1963). Slater (1965) has recently derived full matrix representations for a number of space groups. In the present paper we present tables which, in conjunction with McWeeny's (1963) tables for the point groups, give full matrix representations of all space groups and double space groups.

The method employed is that of ray representations introduced by Weyl (1931) and developed for application to the space groups by Döring (1959). This appears to the author to be the most efficient way of obtaining matrix representations for all 230 space groups without resorting to tables of inordinate length.

When this work was completed attention was drawn (J. P. Dahl, private communication) to a publication by Kovalev (1961) which lists, apart from a gauge transformation, explicit matrices for all irreducible representations of all space groups and double space groups. The relationship of Kovalev's method and tables to those of the present paper is discussed in § 13.

2. RAY REPRESENTATIONS OF FINITE GROUPS

DEFINITION. A ray (or multiplier) representation $\Gamma(a_n)$ of a finite group G with elements $a_1 = e, a_2 \dots a_g$ is a mapping of the elements of G onto a set of non-singular matrices $\Gamma(a_n)$

$$a_n \rightarrow \Gamma(a_n),$$

which satisfies the conditions $\Gamma(a_m) \Gamma(a_n) = \lambda(a_m, a_n) \Gamma(a_m a_n)$ (2.1) for all elements a_m, a_n of G .

In equation (2.1) $\lambda(a_m, a_n)$ is a complex number, which is assumed to be non-zero for all a_m, a_n . The set of numbers $\lambda(a_m, a_n)$ is called the factor system of the ray representation.

The vector representations of G are ray representations with the trivial factor system $\lambda(a_m, a_n) = 1$ for all a_m, a_n of G .

The terms irreducible and equivalent have the same meaning for ray representations as for vector representations. Equivalent ray representations necessarily have the same factor system.

Let $\Gamma^{(1)}(a_n), \Gamma^{(2)}(a_n), \dots, \Gamma^{(N)}(a_n)$ be a complete set of inequivalent irreducible unitary ray representations of G , each with the same factor system $\lambda(a_m, a_n)$. The basic orthogonality relation for irreducible vector representations is valid also for these ray representations:

$$\sum_{a_n \in G} (\Gamma_{ij}^{(\alpha)}(a_n))^* \Gamma_{kl}^{(\beta)}(a_n) = \frac{g}{l_\alpha} \delta_{\alpha\beta} \delta_{ik} \delta_{jl}, \quad (2.2)$$

where l_α is the dimensionality of the ray representation $\Gamma^{(\alpha)}$.

Putting $i = j, k = l$ in equation (2.2) and summing over i and k we obtain the orthogonality relation for the characters

$$\sum_{a_n \in G} (\chi^{(\alpha)}(a_n))^* \chi^{(\beta)}(a_n) = g \delta_{\alpha\beta}, \quad (2.3)$$

where

$$\chi^{(\alpha)}(a_n) = \sum_{i=1}^{l_\alpha} \Gamma_{ii}^{(\alpha)}(a_n).$$

Again, as for vector representations, the number of times n_α that the irreducible ray representation $\Gamma^{(\alpha)}$ is contained in a reducible representation Γ with character χ (and the same factor system $\lambda(a_m, a_n)$ as $\Gamma^{(\alpha)}$) is given by the equation

$$n_\alpha = \frac{1}{g} \sum_{a_n \in G} (\chi^{(\alpha)}(a_n))^* \chi(a_n). \quad (2.4)$$

By considering the regular representation we obtain the useful relation

$$\sum_{\alpha=1}^N l_\alpha^2 = g. \quad (2.5)$$

The derivation of these results is exactly parallel to that for vector representations (Weyl 1931; Wigner 1959). There are two reasons why these results apply without change to ray representations:

(i) Schur's lemma applies to any collection of irreducible matrices and hence to ray as well as vector representations.

(ii) The complex conjugation in equations (2.2), (2.3) and (2.4) leads to cancellation of the elements $\lambda(a_m, a_n)$ of the factor system from these equations.†

When Kronecker products are formed from ray representations attention must be paid to changes in the factor system. If $\Gamma_1(a_n)$, $\Gamma_2(a_n)$ are ray representations of G with factor systems $\lambda_1(a_m, a_n)$, $\lambda_2(a_m, a_n)$ respectively, then the Kronecker product

$$\Gamma(a_n) = \Gamma_1(a_n) \times \Gamma_2(a_n)$$

forms a ray representation of G with the factor system

$$\lambda(a_m, a_n) = \lambda_1(a_m, a_n) \lambda_2(a_m, a_n).$$

Two different factor systems $\lambda(a_m, a_n)$, $\lambda'(a_m, a_n)$ are said to be associated if there exists a set of numbers $\mu(a_n)$ such that

$$\lambda'(a_m, a_n) = \frac{\mu(a_m) \mu(a_n)}{\mu(a_m a_n)} \lambda(a_m, a_n). \quad (2.6)$$

The corresponding transformation of ray representations $\Gamma(a_m)$, $\Gamma'(a_n)$ with factor systems λ , λ' is called a gauge transformation (Weyl 1931),

$$\Gamma'(a_n) = \mu(a_n) \Gamma(a_n). \quad (2.7)$$

Just as similarity transformations may be used to relate all irreducible vector representations of G to a finite set of inequivalent ones, so gauge transformations lead to a finite set of non-associated factor systems. Two ray representations related by any combination of similarity and gauge transformations are said to be projective equivalent or p -equivalent.

As Weyl shows the non-associated factor systems of any group may be obtained from the

† This cancellation does not occur for certain alternative forms of the orthogonality relations for vector representations. For example, the relation

$$\sum_{a_n} \chi^{(\alpha)}(a_n) \chi^{(\beta)}(a_n^{-1}) = g \delta_{\alpha\beta},$$

valid for vector representations, becomes for ray representations

$$\sum_{a_n} [\lambda(a_n, a_n^{-1})]^{-1} \chi^{(\alpha)}(a_n) \chi^{(\beta)}(a_n^{-1}) = g \delta_{\alpha\beta}.$$

However, we shall not have occasion to use these alternative forms.

group structure. In particular he shows that a ray representation of any cyclic group is always associated with a vector representation; that is, for any possible factor system $\lambda(a_m, a_n)$ we can find numbers $\mu(a_n)$ such that

$$\lambda'(a_m, a_n) = \frac{\mu(a_m)\mu(a_n)}{\mu(a_m a_n)} \lambda(a_m, a_n) \equiv 1. \quad (2.8)$$

There are, therefore, no multidimensional irreducible ray representations of cyclic groups. There are, however, some Abelian groups which do have multidimensional irreducible ray representations.

3. RAY REPRESENTATIONS OF POINT GROUPS

We have seen in §2 that for certain point groups the introduction of ray representations leads to nothing essentially new; for these groups any possible representation is associated with an ordinary vector representation.

For other point groups this is not the case; there are ray representations which cannot be associated with vector representations. These groups have been considered by Döring (1959), who finds that among the 32 point groups there are 12 non-isomorphic groups which possess non-trivial ray representations. Döring lists the non-associated factor systems for these 12 groups and the characters of the irreducible ray representations.

Döring's tables have been expanded to give full matrix representations. These expanded tables A 1 to A 11 are given in the appendix to this paper.

4. SPACE GROUPS

The general theory of space groups and their representations has been reviewed by Koster (1957) and we follow his notation and conventions with minor exceptions, which are stated explicitly.

A space group G is an infinite discrete group of point transformations of the form $\{a|\mathbf{t}\}$. The transform \mathbf{x}' of a general point (vector) \mathbf{x} by $\{a|\mathbf{t}\}$ is defined by the equation

$$\mathbf{x}' = \{a|\mathbf{t}\}\mathbf{x} = a\mathbf{x} + \mathbf{t}. \quad (4.1)$$

In a fixed Cartesian coordinate system \mathbf{x}' , \mathbf{x} and \mathbf{t} are represented by 3×1 column matrices and a is represented by a real orthogonal 3×3 matrix. The vector \mathbf{t} is called the translational part of the transformation (4.1) and a is called the rotational part.

The product of two elements $\{a|\mathbf{t}\}$, $\{b|\mathbf{s}\}$ of G is defined by transforming a general vector \mathbf{x} successively by $\{b|\mathbf{s}\}$ and $\{a|\mathbf{t}\}$,

$$\{a|\mathbf{t}\}\{b|\mathbf{s}\}\mathbf{x} = \{a|\mathbf{t}\}(\{b|\mathbf{s}\}\mathbf{x}). \quad (4.2)$$

From equation (4.2) we obtain the product rule

$$\{a|\mathbf{t}\}\{b|\mathbf{s}\} = \{ab|\mathbf{as} + \mathbf{t}\}. \quad (4.3)$$

As Koster shows, any group of transformations of the form (4.1) possesses an invariant subgroup \mathcal{T} of pure translations $\{e|\mathbf{t}\}$, where e is the identity rotation; space groups are characterized by the form of this subgroup \mathcal{T} . All the pure translations of a space group, called primitive translations, are of the form

$$\{e|\mathbf{t}\} = \{e|\mathbf{R}_n\}, \quad (4.4)$$

where

$$\mathbf{R}_n = n_1 \mathbf{t}_1 + n_2 \mathbf{t}_2 + n_3 \mathbf{t}_3.$$

Here n_1, n_2 and n_3 are integers and $\mathbf{t}_1, \mathbf{t}_2, \mathbf{t}_3$ are three linearly independent translations, called basic primitive translations. The periodic collection of points generated by the vectors \mathbf{R}_n is called the lattice. This lattice must be one of the 14 possible Bravais lattices listed by Koster, who also gives the symmetrical unit cell for each lattice.

The rotational parts a_i ($i = 1, \dots, g$) of the transformations (4.1) constitute one of the 32 point groups. This point group G_0 , which for a given space group G must leave the symmetrical unit cell invariant, is not, in general, a subgroup of G . However, G_0 is always isomorphic to the factor group G/\mathcal{T} .

All elements of G which have a rotational part a_i can be written in the form

$$\{a_i | \mathbf{t}\} = \{a_i | \mathbf{v}(a_i) + \mathbf{R}_n\} = \{e | \mathbf{R}_n\} \{a_i | \mathbf{v}(a_i)\}, \quad (4.5)$$

where \mathbf{R}_n runs over all primitive translations. Here $\mathbf{v}(a_i)$ is either zero or a non-primitive translation, which, for each a_i , is usually chosen so that the length of $\mathbf{v}(a_i)$ is as small as possible; $\mathbf{v}(a_i)$ will be referred to as the (minimal) non-primitive translation associated with the rotation a_i . Motions corresponding to non-primitive translations followed by a proper or improper rotation correspond to glide planes and screw axes in a crystal.

We see then that a unique vector $\mathbf{v}(a_i)$, which may be zero, is associated with each element a_i of the point group. We always associate a primitive translation \mathbf{R}_n with the identity rotation $a = e$ so that $\mathbf{v}(e) = 0$.

Space groups may be divided into two types on the basis of the vectors $\mathbf{v}(a_i)$. The first are those for which $\mathbf{v}(a_i) = 0$ for all a_i . These are the so-called symmorph space groups of which there are 73. For each element a_i of the point group G_0 there is an element $\{a_i | 0\}$ in the symmorph space group G . From equation (4.2) we have

$$\{a_i | 0\} \{a_j | 0\} = \{a_i a_j | 0\},$$

so that those elements of G of the form $\{a_i | 0\}$ constitute a subgroup isomorphic with G_0 . Thus we can characterize the symmorph space groups by saying that they contain the entire point group as a subgroup.

In the remaining 157 space groups, $\mathbf{v}(a_i)$ cannot be taken as zero for all a_i simultaneously. For a non-symmorph space group G of this type, the set of elements

$$\{a_i | \mathbf{v}(a_i)\} \quad (i = 1, \dots, g) \quad (4.6)$$

does not constitute a group. This set of elements, which will be referred to as the reduced set $\{G_0\}$ of the space group G , plays an important role in the derivation of the representations. The element (4.6) of the reduced set will sometimes be abbreviated to $\{a_i\}$. We note that the translational part of the transformation $\{a_i\}$ is not necessarily zero.

The product of two elements $\{a_i | \mathbf{v}(a_i)\}, \{a_j | \mathbf{v}(a_j)\}$ of the reduced set $\{G_0\}$ may be found from equation {4.3},

$$\{a_i | \mathbf{v}(a_i)\} \{a_j | \mathbf{v}(a_j)\} = \{a_i a_j | a_i \mathbf{v}(a_j) + \mathbf{v}(a_i)\}. \quad (4.7)$$

Now from equation (4.5) we must have

$$a_i \mathbf{v}(a_j) + \mathbf{v}(a_i) = \mathbf{v}(a_i a_j) + \mathbf{R}_n(i, j) \quad (4.8)$$

where $\mathbf{R}_n(i, j)$ is a primitive translation depending on i and j .

$$\begin{aligned} \text{Therefore } \{a_i | \mathbf{v}(a_i)\} \{a_j | \mathbf{v}(a_j)\} &= \{a_i a_j | \mathbf{v}(a_i a_j) + \mathbf{R}_n(i, j)\} \\ &= \{e | \mathbf{R}_n(i, j)\} \{a_i a_j | \mathbf{v}(a_i a_j)\}, \end{aligned} \quad (4.9)$$

or in the abbreviated notation

$$\{a_i\} \{a_j\} = \{e | \mathbf{R}_n(i, j)\} \{a_i a_j\}. \quad (4.10)$$

The fact that the reduced set $\{G_0\}$ is not, in general, a group is apparent from equation (4.10). Only if $\mathbf{R}_n(i, j)$ happens to be zero will the product of two elements in $\{G_0\}$ give a result in $\{G_0\}$; otherwise the result will differ from an element of $\{G_0\}$ by a factor which is an element of the subgroup \mathcal{F} of pure translations.

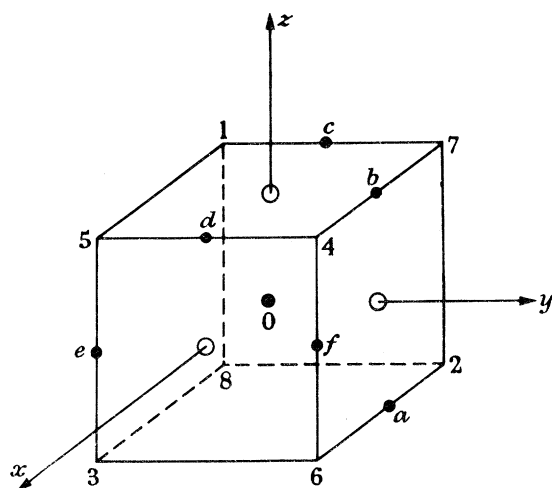


FIGURE 1. Diagram for the point group O_h and its subgroups.

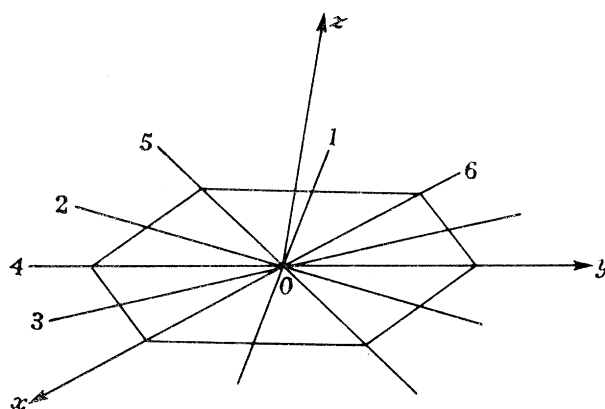


FIGURE 2. Diagram for the point group D_{6h} and its subgroups.

The basic equation (4.10) will enable us to relate the vector representations of space groups and double space groups to the ray representations of the point groups. In setting up this relation it is important to have a quick, simple method for evaluating products of space group elements such as appear in equation (4.7). This may be achieved using a multiplication table to evaluate the products $a_i a_j$ and a diagram to evaluate the products $a_i \mathbf{v}(a_j)$. Since every point group is a subgroup of either O_h or D_{6h} , two multiplication tables and two diagrams suffice. These are given in tables 1 and 2 and figures 1 and 2.

Three notations for the point group element are given at the top of tables 1 and 2:

(i) A simple subscript notation $a_1 = e$, $a_2 \dots a_g$ (b 's for table 2). This notation enables products $a_i a_j$ to be obtained immediately from the table entries; these entries give the subscript k of the product ($a_i a_j = a_k$). The bars appearing over certain entries should be ignored here; they refer to the double groups (cf. § 7).

(ii) A geometrical notation related to figures 1 and 2. Here each rotation is a positive rotation (right hand screw) about the axis from the origin O to the appropriate point at the edge of the diagram. The angle of rotation is always less than or equal to π . This notation and the diagrams enable us to write down all products $a_i \mathbf{v}(a_j)$ immediately. For example, if $\mathbf{v}(a_j)$ is a non-primitive translation in the direction 4 (figure 1), $a_{14} \mathbf{v}(a_j)$ is a non-primitive

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translation in the direction 5. This notation also enables us to identify the matrices of the vector representations of the point groups given by McWeeny (1963).

(iii) The coordinates of equivalent positions. These are the vectors that are obtained by transforming a general column vector (x, y, z) by all elements a_i (or b_i) of the point group (cf. equation (4.1)). This notation enables us to make use of the *International tables for X-ray crystallography* (1953) referred to hereafter as the *International tables*. The listing of equivalent

TABLE 1. EQUIVALENT POSITIONS, GEOMETRICAL IDENTIFICATION AND MULTIPLICATION
TABLE FOR THE POINT GROUP O_h AND ITS SUBGROUPS

The entries give the subscript k such that $a_i a_j = a_k$. The bars indicate the factor system for spin representations.

Equivalent positions

x	x	\bar{x}	\bar{x}	z	\bar{z}	z	\bar{z}	y	\bar{y}	\bar{y}	y	x	x	\bar{z}	z	y	\bar{y}	\bar{x}	\bar{x}	\bar{z}	z	\bar{y}	y
y	\bar{y}	y	\bar{y}	x	\bar{x}	\bar{x}	x	z	z	\bar{z}	\bar{z}	y	\bar{y}	y	\bar{x}	x	x	\bar{z}	\bar{z}	\bar{y}	y	\bar{x}	x
z	\bar{z}	\bar{z}	z	y	\bar{y}	\bar{y}	y	x	\bar{x}	x	\bar{x}	y	\bar{y}	x	\bar{x}	z	z	\bar{y}	y	\bar{x}	x	\bar{z}	\bar{z}

Geometrical identification (figure 1) and multiplication table

$i \setminus j$	e	C_2^x	C_2^y	C_2^z	$C_3^{(4)}$	$C_3^{(3)}$	$C_3^{(2)}$	$C_3^{(1)}$	$C_3^{(8)}$	$C_3^{(7)}$	$C_3^{(5)}$	$C_3^{(6)}$	C_4^{-x}	C_4^x	C_4^{-y}	C_4^y	C_4^{-z}	C_4^z	C_2^a	C_2^b	C_2^c	C_2^d	C_2^e	C_2^f
	1	2	3	4	5	6	7	8	9	10	11	12	13	14	15	16	17	18	19	20	21	22	23	24
1	1	2	3	4	5	6	7	8	9	10	11	12	13	14	15	16	17	18	19	20	21	22	23	24
2	2	1	4	3	7	8	5	6	12	11	10	9	14	13	21	22	24	23	20	19	15	16	18	17
3	3	4	1	2	8	7	6	5	10	9	12	11	20	19	16	15	23	24	14	13	22	21	17	18
4	4	3	2	1	6	5	8	7	11	12	9	10	19	20	22	21	18	17	13	14	16	15	24	23
5	5	8	6	7	9	12	10	11	1	4	2	3	18	24	14	20	16	22	23	17	19	13	21	15
6	6	7	5	8	11	10	12	9	4	1	3	2	17	23	20	14	21	15	24	18	13	19	16	22
7	7	6	8	5	12	9	11	10	2	3	1	4	23	17	13	19	22	16	18	24	20	14	15	21
8	8	5	7	6	10	11	9	12	3	2	4	1	24	18	19	13	15	21	17	23	14	20	22	16
9	9	11	12	10	1	3	4	2	5	7	8	6	22	15	24	17	20	13	21	16	23	18	19	14
10	10	12	11	9	3	1	2	4	8	6	5	7	21	16	18	23	13	20	22	15	17	24	14	19
11	11	9	10	12	4	2	1	3	6	8	7	5	15	22	23	18	14	19	16	21	24	17	13	20
12	12	10	9	11	2	4	3	1	7	5	6	8	16	21	17	24	19	14	15	22	18	23	20	13
13	13	14	19	20	16	15	22	21	24	23	18	17	2	1	8	7	9	10	4	3	6	5	11	12
14	14	13	20	19	22	21	16	15	17	18	23	24	1	2	6	5	12	11	3	4	8	7	10	9
15	15	22	16	21	18	23	17	24	20	13	19	14	9	11	3	1	6	8	12	10	2	4	7	5
16	16	21	15	22	24	17	23	18	13	20	14	19	10	12	1	3	7	5	11	9	4	2	6	8
17	17	23	24	18	14	20	19	13	22	16	15	21	7	6	9	12	4	1	8	5	10	11	3	2
18	18	24	23	17	20	14	13	19	15	21	22	16	8	5	11	10	1	4	7	6	12	9	2	3
19	19	20	13	14	21	22	15	16	23	24	17	18	3	4	7	8	11	12	1	2	5	6	9	10
20	20	19	14	13	15	16	21	22	18	17	24	23	4	3	5	6	10	9	2	1	7	8	12	11
21	21	16	22	15	23	18	24	17	19	14	20	13	12	10	4	2	8	6	9	11	1	3	5	7
22	22	15	21	16	17	24	18	23	14	19	13	20	11	9	2	4	5	7	10	12	3	1	8	6
23	23	17	18	24	19	13	14	20	21	15	16	22	6	7	10	11	2	3	5	8	9	12	1	4
24	24	18	17	23	13	19	20	14	16	22	21	15	5	8	12	9	3	2	6	7	11	10	4	1

Inversion a'_i commutes with all a_i , $a_i'^2 = e$, $a_i a'_i = a'_i$.

positions in these tables gives the non-primitive translation associated with each element of the point group. Since non-primitive unit cells are used for many space groups in the *International tables*, the non-primitive translations obtained directly from the tables may not be minimal; to obtain minimal non-primitive translations, suitable primitive translations of the relevant lattice must be added. A change of origin may also be used in some cases to simplify the minimal non-primitive translations.

We note that in figure 2 and table 2 the oblique axes x, y, z of the *International tables* are used rather than the orthogonal axes which appear in the corresponding diagram of Koster (1957).

TABLE 2. EQUIVALENT POSITIONS, GEOMETRICAL IDENTIFICATION AND MULTIPLICATION TABLE FOR THE POINT GROUP D_{6h} AND ITS SUBGROUPS

The entries give the subscript k such that $b_i b_j = b_k$. The bars indicate the factor system for spin representations.

Equivalent positions†

x	\bar{x}	\bar{y}	$y-x$	$x-y$	y	x	$y-x$	\bar{y}	\bar{x}	y	$x-y$
y	\bar{y}	$x-y$	\bar{x}	x	$y-x$	$x-y$	\bar{y}	\bar{x}	$y-x$	x	\bar{y}
z	z	z	z	z	z	\bar{z}	\bar{z}	\bar{z}	\bar{z}	\bar{z}	\bar{z}

Geometrical identification (figure 2) and multiplication table

$i \backslash j$	e	C_2^z	C_3^z	C_3^{-z}	C_6^z	C_6^{-z}	$C_2^{(1)}$	$C_2^{(2)}$	$C_2^{(3)}$	$C_2^{(4)}$	$C_2^{(5)}$	$C_2^{(6)}$
1	1	2	3	4	5	6	7	8	9	10	11	12
2	2	$\bar{1}$	$\bar{6}$	5	4	3	10	$\bar{12}$	$\bar{11}$	7	9	8
3	3	$\bar{6}$	4	1	2	5	8	9	$\bar{7}$	$\bar{12}$	10	11
4	4	5	1	$\bar{3}$	6	$\bar{2}$	$\bar{9}$	7	8	11	12	$\bar{10}$
5	5	$\bar{4}$	2	6	3	1	11	10	$\bar{12}$	9	8	7
6	6	3	5	2	1	4	12	11	10	8	7	$\bar{9}$
7	7	$\bar{10}$	9	8	12	11	$\bar{1}$	$\bar{4}$	3	2	$\bar{6}$	$\bar{5}$
8	8	12	7	9	11	10	$\bar{3}$	$\bar{1}$	$\bar{4}$	$\bar{6}$	$\bar{5}$	$\bar{2}$
9	9	11	8	7	10	$\bar{12}$	4	$\bar{3}$	$\bar{1}$	$\bar{5}$	$\bar{2}$	6
10	10	7	11	$\bar{12}$	8	9	$\bar{2}$	$\bar{5}$	$\bar{6}$	$\bar{1}$	$\bar{3}$	4
11	11	$\bar{9}$	12	10	7	8	$\bar{5}$	$\bar{6}$	2	4	$\bar{1}$	$\bar{3}$
12	12	$\bar{8}$	$\bar{10}$	11	9	7	$\bar{6}$	2	5	3	4	$\bar{1}$

Inversion b'_1 commutes with all b_i , $b_1'^2 = e$, $b_i b_1' = b_i'$.

† The oblique axes of the *International tables* (1953) for the hexagonal system are used here (cf. figure 2).

A space group G is most economically specified by giving:

(i) the basic translations $\mathbf{t}_1, \mathbf{t}_2$ and \mathbf{t}_3 which generate the subgroup \mathcal{T} of pure translations, that is, the Bravais lattice;

(ii) the point group G_0 of order g ;

(iii) the non-primitive translations associated in G with a set of generators of G_0 .

For all non-cyclic groups, sets of generators (a, b, \dots) are given at the head of tables A 0 to A 11 in the appendix to this paper. The geometric identification of these generators and the algebraic relations they satisfy are also given. From tables A 0 to A 11 we see that, even in the most complex case (O_h), only five generators and the corresponding non-primitive translations need be specified. The geometric identification of the generators enables us to relate them to the elements (a_1, a_2, \dots) of table 1 or (b_1, b_2, \dots) of table 2. In the case of O_h , for example, we have† $a = a_2, b = a_3, c = a_5, d = a_{23}, i = a'_1$.

Once this identification has been made, equation (4.3) table 1 (or 2) and figure 1 (or 2) enables us to write down immediately any products of the generators $\{a\}, \{b\}, \dots$ of the reduced set $\{G_0\}$. In this way we may obtain:

† This choice of generators is not unique.

(i) The non-primitive translation associated with each element of the point group G_0 in the reduced set $\{G_0\}$. Alternatively, all these non-primitive translations may be obtained directly from the *International tables*.

(ii) The primitive translation $\mathbf{R}_n(i, j)$ associated with the product $\{a_i\}\{a_j\}$ of any two elements of the reduced set $\{G_0\}$ (cf. equation (4.10)). One could, in fact, prepare a complete table of the g^2 factors $\{e|\mathbf{R}_n(i, j)\}$ for all possible products $\{a_i\}\{a_j\}$. This is unnecessary, however, since relatively few products are needed to identify the representations (cf. § 9). It is simpler to use table 1 (or 2) and figure 1 (or 2) to evaluate any required product.

5. GENERAL THEORY OF THE REPRESENTATIONS OF SPACE GROUPS

We follow Koster (1957). To describe the irreducible representations of a space group G we need three concepts: the reciprocal lattice, the Brillouin zone and the group (\mathcal{H}) of the \mathbf{k} vector.

The reciprocal lattice is generated by three basic vectors $\mathbf{b}_1, \mathbf{b}_2, \mathbf{b}_3$ defined by

$$\mathbf{t}_i \cdot \mathbf{b}_j = 2\pi\delta_{ij} \quad (i, j = 1, 2, 3). \quad (5.1)$$

Here $\mathbf{t}_1, \mathbf{t}_2, \mathbf{t}_3$ are the basic primitive translations which generate the subgroup \mathcal{T} of pure translations. The points \mathbf{K}_q of the reciprocal lattice are given by

$$\mathbf{K}_q = q_1 \mathbf{b}_1 + q_2 \mathbf{b}_2 + q_3 \mathbf{b}_3, \quad (5.2)$$

where q_1, q_2, q_3 are any integers.

The Brillouin zone is the symmetrical unit cell of the reciprocal lattice; its interior consists of all points nearer to the origin of the reciprocal lattice than to any other lattice point. It follows that no two points in the interior of the Brillouin zone are equivalent, that is, differ by a vector of the reciprocal lattice, whereas any point on the surface of the Brillouin zone is equivalent to at least one other point on the surface.

Koster shows that a complete set of inequivalent irreducible representations of the subgroup \mathcal{T} of pure translations $\{e|\mathbf{R}_n\}$ is given by†

$$\exp(-i\mathbf{k} \cdot \mathbf{R}_n), \quad (5.3)$$

where the vector \mathbf{k} ranges over the interior and surface of the Brillouin zone. Since equivalent points on the surface of the zone yield equivalent representations of \mathcal{T} , each set of equivalent surface points contributes only one irreducible representation. All these representations are one-dimensional since \mathcal{T} is Abelian.

For each \mathbf{k} vector within or on the surface of the Brillouin zone certain elements $\{b|\mathbf{t}\}$ of the space group G will have the property

$$\exp(i\mathbf{b}\mathbf{k} \cdot \mathbf{R}_n) = \exp(i\mathbf{k} \cdot \mathbf{R}_n) \quad (5.4)$$

for all primitive translations \mathbf{R}_n . Elements with the property (5.4) form a subgroup \mathcal{H} of G , called the group of the wave vector \mathbf{k} (or \mathbf{k} vector). Clearly for any \mathbf{k} vector, \mathcal{H} is a space group which includes the entire group \mathcal{T} of pure translations.

† The vector \mathbf{k} here is the negative of Koster's (1957). Either choice gives a consistent mathematical theory, but the physical interpretation of \mathbf{k} as a quasi-momentum requires a minus sign in equation (5.3) and a plus sign in the expression for a Bloch function (cf. § 8, and Altmann & Cracknell (1965)).

The condition (5.4) is equivalent to

$$b\mathbf{k} = \mathbf{k} + \mathbf{K}_q, \quad (5.5)$$

where \mathbf{K}_q is a vector of the reciprocal lattice. Now if \mathbf{k} is in the interior of the Brillouin zone so is $b\mathbf{k}$. Thus for interior points of the zone the condition (5.5) defining \mathcal{K} reduces to

$$b\mathbf{k} = \mathbf{k} \quad (5.6)$$

since no two interior points of the Brillouin zone can differ by a non-zero vector of the reciprocal lattice.

We are now in a position to state the basic theorems given by Koster (1957).

THEOREM 1. *Any irreducible representation of a space group G , in standard form, induces an irreducible representation of \mathcal{K} , in which the pure translations $\{e | \mathbf{R}_n\}$ are represented by the diagonal matrices*

$$\exp(-i\mathbf{k} \cdot \mathbf{R}_n) I_d. \quad (5.7)$$

Here d is the dimensionality of the irreducible representation of \mathcal{K} and I_d is the $d \times d$ unit matrix.

THEOREM 2 (converse of 1). *Any irreducible representation of \mathcal{K} , the group of the wave vector \mathbf{k} , in which the pure translations $\{e | \mathbf{R}_n\}$ are represented by the diagonal matrices (5.7) may be extended to an irreducible representation of the entire space group G .*

The standard form of the representations and the procedure for extending the representations of \mathcal{K} are fully described by Koster. The process of extension involves the resolution of G into left cosets with respect to the subgroup \mathcal{K} . Once this resolution has been effected, the matrices representing the elements of G may be written down immediately in terms of those representing the elements of \mathcal{K} .

6. IRREDUCIBLE REPRESENTATIONS OF \mathcal{K} AS RAY REPRESENTATIONS OF POINT GROUPS

The theorems of §5 reduce the problem of finding all irreducible representations of a space group G to that of finding, for each \mathbf{k} vector of the Brillouin zone,† those irreducible representations of \mathcal{K} in which the pure translations appear in the form (5.7).

To obtain these representations of \mathcal{K} we consider the point group $G_0(k)$ formed by the rotational parts of the elements of \mathcal{K} . We note that, in general, $G_0(k)$ is not a subgroup of \mathcal{K} . We consider also the reduced set $\{G_0(k)\}$ of the space group \mathcal{K} consisting of the elements

$$\{b\} = \{b | \mathbf{v}(b)\}. \quad (6.1)$$

Here b runs through the g_k elements of $G_0(k)$, and $\mathbf{v}(b)$ is the minimal non-primitive translation associated with b in the space groups G and \mathcal{K} .

† To obtain all distinct representations of G , one need not consider the whole Brillouin zone but only a set of \mathbf{k} vectors such that no two vectors \mathbf{k} , \mathbf{k}' of the set satisfy the relation

$$\mathbf{k}' = a\mathbf{k} + \mathbf{K}_j.$$

Here a is any element of the point group G_0 and \mathbf{K}_j is any vector of the reciprocal lattice. The set defined in this way (the fundamental region of reciprocal space) constitutes a fraction $1/g$ of the whole Brillouin zone, where g is the order of G_0 (Koster 1957).

Let $D(\{b | \mathbf{t}\})$ denote an irreducible representation of \mathcal{K} in which the pure translations appear in the form (5.7). For any two elements $\{b_i\}, \{b_j\}$ of the reduced set $\{G_0(k)\}$ we have

$$\begin{aligned} D(\{b_i\}) D(\{b_j\}) &= D(\{b_i\} \{b_j\}) \\ &= D(\{e | \mathbf{R}_n(i, j)\} \{b_i b_j\}) \\ &= D(\{e | \mathbf{R}_n(i, j)\}) D(\{b_i b_j\}). \end{aligned} \quad (6.2)$$

Therefore
$$D(\{b_i\}) D(\{b_j\}) = \exp(-\mathbf{i}\mathbf{k} \cdot \mathbf{R}_n(i, j)) D(\{b_i b_j\}). \quad (6.3)$$

Here we have used equations (4.10), (5.7) and the fact that the matrices D provide a representation of \mathcal{K} .

Comparing equation (6.3) with equation (2.1) we see that the matrices $D(\{b_i\})$ representing the elements $\{b_i\}$ of the reduced set $\{G_0(k)\}$ provide a ray representation of the point group $G_0(k)$ with the factor system

$$\lambda(b_i, b_j) = \exp(-\mathbf{i}\mathbf{k} \cdot \mathbf{R}_n(i, j)). \quad (6.4)$$

This ray representation of $G_0(k)$ is clearly irreducible.

We have therefore established the following result.

THEOREM 3. *An irreducible representation of \mathcal{K} in which the pure translations are represented by the diagonal matrices (5.7) induces† an irreducible ray representation of the point group $G_0(k)$ with the factor system*

$$\lambda(b_i, b_j) = \exp(-\mathbf{i}\mathbf{k} \cdot \mathbf{R}_n(i, j)). \quad (6.4)$$

Here $\mathbf{R}_n(i, j)$ is the primitive translation given by

$$\{b_i\} \{b_j\} = \{e | \mathbf{R}_n(i, j)\} \{b_i b_j\},$$

that is from equation (4.8)

$$\mathbf{R}_n(i, j) = b_i \mathbf{v}(b_j) + \mathbf{v}(b_i) - \mathbf{v}(b_i b_j). \quad (6.5)$$

Conversely, we have

THEOREM 4. *An irreducible ray representation $D(\{b_i\})$ of the point group $G_0(k)$ with the factor system (6.4), (6.5) may be extended† to give an irreducible representation of the space group \mathcal{K} , in which the pure translations are represented by the diagonal matrices (5.7).*

For a general element $\{b | \mathbf{t}\}$ of \mathcal{K} the extension† of the representation is provided by the equations

$$\begin{aligned} D(\{b | \mathbf{t}\}) &= D(\{b | \mathbf{v}(b) + \mathbf{R}_m\}) \\ &= \exp(-\mathbf{i}\mathbf{k} \cdot \mathbf{R}_m) D(\{b\}). \end{aligned} \quad (6.6)$$

Theorems 1 to 4 enable us to construct complete sets of full matrix representations of all 230 space groups from the ray representations of the point groups given in the appendix and the vector representations of the point groups given by McWeeny (1963). In some cases one must carry out a preliminary gauge transformation of the form given by equations (2.6) and (2.7) in order to associate the factor system (6.4), either with the trivial factor system $\lambda(b_i, b_j) = 1$ of a vector representation; or with one of the factor systems listed explicitly in tables A 1 to A 11. The derivation of these gauge transformations is described in § 9.

† Since $G_0(k)$ is not a subgroup of \mathcal{K} the terms ‘induce’ and ‘extend’ are, perhaps, not strictly appropriate. However, their meaning is clear from the derivation of theorem 3.

For symmorphic space groups, and for \mathbf{k} vectors in the interior of the Brillouin zone for non-symmorphic groups, the simplifications given by Koster (1957) appear naturally in the present treatment. For symmorphic groups all the non-primitive translations appearing in equation (6.5) are zero. Consequently, $\mathbf{R}_n(i, j) = 0$ for all values of i and j and the factor system (6.4) becomes the trivial factor system $\lambda(b_i, b_j) \equiv 1$. The irreducible representations of \mathcal{K} are therefore given by

$$D(\{b | \mathbf{t}\}) = \exp(-i\mathbf{k} \cdot \mathbf{t}) \Gamma(b), \quad (6.7)$$

where $\Gamma(b)$ is a vector representation of $G_0(k)$.

For points in the interior of the Brillouin zone all elements b_i of $G_0(k)$ leave \mathbf{k} invariant (equation (5.6)). Consequently, from equations (6.4) and (6.5) we have

$$\begin{aligned} \lambda(b_i, b_j) &= \exp(-i\mathbf{k} \cdot (b_i \mathbf{v}(b_j) + \mathbf{v}(b_i) - \mathbf{v}(b_i b_j))) \\ &= \exp(-i b_i^{-1} \mathbf{k} \cdot \mathbf{v}(b_j)) \exp(-i\mathbf{k} \cdot \mathbf{v}(b_i)) \exp(i\mathbf{k} \cdot \mathbf{v}(b_i b_j)) \\ &= \frac{\exp(-i\mathbf{k} \cdot \mathbf{v}(b_j)) \exp(-i\mathbf{k} \cdot \mathbf{v}(b_i))}{\exp(-i\mathbf{k} \cdot \mathbf{v}(b_i b_j))}. \end{aligned} \quad (6.8)$$

Therefore, from equation (2.6) we see that the gauge transformation

$$D'(b_i) = \exp(i\mathbf{k} \cdot \mathbf{v}(b_i)) D(\{b_i\}) \quad (6.9)$$

associates the factor system (6.8) with the trivial factor system $\lambda(b_i, b_j) \equiv 1$.

The matrix representing a general element $\{b | \mathbf{t}\}$ of \mathcal{K} is from equation (6.6), (6.9)

$$\begin{aligned} D(\{b | \mathbf{t}\}) &= \exp(-i\mathbf{k} \cdot \mathbf{R}_m) \exp(-i\mathbf{k} \cdot \mathbf{v}(b)) D'(b) \\ &= \exp(-i\mathbf{k} \cdot \mathbf{t}) D'(b). \end{aligned} \quad (6.10)$$

The final result (6.10) is identical with (6.7) since the matrices $D'(b)$ provide a vector representation of $G_0(k)$.

7. SPIN REPRESENTATIONS

The effects of electron spin are usually incorporated into the representation theory of point and space groups by the following device (Wigner 1959). The full rotation group R_3 possesses, in addition to the usual one-valued vector representations $\mathcal{D}_0, \mathcal{D}_1, \dots$, certain two-valued representations $\mathcal{D}_{\frac{1}{2}}, \mathcal{D}_{\frac{3}{2}}, \dots$. These two-valued representations of R_3 are obtained as one-valued vector representations of the covering group of R_3 , which is the group U_2 of 2×2 unitary transformations. When applied to a point group G_0 with elements $a_1 = e, a_2, \dots, a_g$ this approach leads to a consideration of the so-called double group G_{0d} with elements $a_1 = e, a_2, \dots, a_g, \bar{a}_1, \bar{a}_2, \dots, \bar{a}_g$ (Koster 1957). The representations of G_{0d} are of two types:

(i) Those derived from the one-valued vector representations of G_0 . The matrices Γ of these representations satisfy

$$\Gamma(\bar{a}_i) = \Gamma(a_i). \quad (7.1)$$

(ii) The so-called additional representations of G_{0d} . Here the representation matrices Γ_s satisfy

$$\Gamma_s(\bar{a}_i) = -\Gamma_s(a_i). \quad (7.2)$$

As Weyl (1931) points out, the theory of ray representations provides an alternative treatment of electron spin which is in many ways simpler than the usual one. Here the spin representations of a point group G_0 are obtained as one-valued ray representations of G_0

with a factor system λ_s given by the standard spin representation $\mathcal{D}_{\frac{1}{2}}$ of the full rotation group.

In specifying the elements of G_0 it is necessary to distinguish between rotations ϕ and $2\pi - \phi$ about the same axis. We adhere to the conventions given in §4 (figures 1 and 2). All rotations are positive rotations (right-hand screw) about axes directed away from the origin through angles less than or equal to π .

With these conventions, the matrix for the rotation (ϕ, \mathbf{n}) , through an angle ϕ about the axis \mathbf{n} in the standard spin representation $\mathcal{D}_{\frac{1}{2}}$, is given by

$$R_s(\phi, \mathbf{n}) = I \cos \frac{1}{2}\phi - i\boldsymbol{\sigma} \cdot \mathbf{n} \sin \frac{1}{2}\phi \quad (7.3)$$

where
$$I = \begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix}, \quad \sigma_x = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}, \quad \sigma_y = \begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix}, \quad \sigma_z = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}.$$

For an improper rotation a'_i we have $R_s(a'_i) = R_s(a_i)$.

The matrices (7.3) were constructed explicitly for all elements of O_h and D_{6h} . By forming products of these matrices the factor systems indicated by the bars in tables 1 and 2 were obtained. If a_k (or b_k) appears unbarred in these tables, this implies

$$R_s(a_i) R_s(a_j) = R_s(a_k), \quad (7.4)$$

i.e.

$$\lambda_s(a_i, a_j) = 1,$$

whereas an entry \bar{a}_k indicates that

$$R_s(a_i) R_s(a_j) = -R_s(a_k), \quad (7.5)$$

i.e.

$$\lambda_s(a_i, a_j) = -1.$$

Since any point group is a subgroup of either O_h or D_{6h} tables 1 and 2 suffice for all 32 point groups. Hence by associating the factor system (7.4), (7.5) obtained from table 1 (or 2) with one appearing explicitly in tables A 0 to A 11 we obtain full matrix spin representations of all the point groups. The required gauge transformations are easily obtained by considering the generators of the point groups (§9). These spin representations $\Gamma_s(a_i)$ of a point group G_0 may immediately be extended to full matrix vector representations (the additional representations) of the double group G_{0d} by using equation (7.2).

The treatment of the double space groups is equally simple. The factor system $\lambda_{ks}(b_i, b_j)$, for the ray representation of $G_0(k)$, which corresponds to a spin representation of the group \mathcal{H} of the \mathbf{k} vector, is given by

$$\lambda_{ks}(b_i, b_j) = \lambda_s(b_i, b_j) \exp(-i\mathbf{k} \cdot \mathbf{R}_n(i, j)). \quad (7.6)$$

That is, to obtain the factor system for a spin representation of \mathcal{H} , we introduce a minus sign on the right-hand side of equation (6.4) whenever the product $b_i b_j$ appears with a bar in table 1 (or 2). Again a gauge transformation may be required to associate the factor system (7.6) with one appearing explicitly in tables A 0 to A 11 (§9).

Finally the ray representations of $G_0(k)$, with and without spin, may be extended using equations (7.1) and (7.2) and theorem 4 to full matrix vector representations of \mathcal{H}_d the double group of the \mathbf{k} vector, and hence by theorem 2 to full matrix vector representations of the double space group G_d .

We note that the separation of the elements of a double group into classes, which is the key to the usual treatment of additional representations (Koster 1957) is unimportant here.

These classes may, of course, be obtained from the final character tables. Two elements belong to the same class if and only if they have the same character in all irreducible representations.

8. PROJECTION OPERATORS AND BASIS FUNCTIONS

Following the convention introduced by Wigner (1959) and Weyl (1931) the transforms of scalar functions of position f and spinor functions g are defined by the linear operators

$$\mathcal{L}_{\{a|\mathbf{t}\}} f(\mathbf{x}) = f(\{a|\mathbf{t}\}^{-1}\mathbf{x}) = f(a^{-1}(\mathbf{x}-\mathbf{t})), \quad (8.1)$$

$$\mathcal{L}_{\{a|\mathbf{t}\}}^s g(\mathbf{x}) = R_s g(\{a|\mathbf{t}\}^{-1}\mathbf{x}). \quad (8.2)$$

Here R_s is the matrix representing the rotation a in the standard spin representation (equation (7.3)) and the inverse transformation $\{a|\mathbf{t}\}^{-1}$ appearing in equation (8.1) has been evaluated explicitly with the aid of equation (4.3).

With this convention the linear operators $\mathcal{L}_{\{a|\mathbf{t}\}}$ form a group isomorphic with the group G . Consequently we may abbreviate $\mathcal{L}_{\{a|\mathbf{t}\}}$ and $\mathcal{L}_{\{a|\mathbf{t}\}}^s$ to $\{a|\mathbf{t}\}$ without risk of confusion.

One of the most useful applications of the full matrices for the irreducible representations of a group is to provide projection operators for basis functions. If $\Gamma^{(\alpha)}(a_n)$ is an irreducible representation of any group G and ψ is an arbitrary function (or vector), then the function (vector)

$$\phi_{ij}^{(\alpha)} = \sum_{a_n \in G} (\Gamma_{ij}^{(\alpha)}(a_n))^* a_n \psi \quad (8.3)$$

is either identically zero or transforms as the i th partner in the representation $\Gamma^{(\alpha)}$ (McWeeny 1963).

If, in equation (8.3), G is taken as \mathcal{K} the group of the wave vector \mathbf{k} , an important simplification arises from the special form (6.6) of the representation matrices.

Thus if

$$\{b|\mathbf{t}\} = \{b|\mathbf{v}(b) + \mathbf{R}_m\} \quad (8.4)$$

is a general element of \mathcal{K} and if

$$D^{(\alpha)}(\{b|\mathbf{t}\}) = \exp(-i\mathbf{k} \cdot \mathbf{R}_m) D^{(\alpha)}(\{b\}) \quad (8.5)$$

is an irreducible representation of \mathcal{K} in standard form, then (8.3) becomes

$$\begin{aligned} \phi_{ij}^{(\alpha)} &= \sum_{\mathcal{K}} D_{ij}^{(\alpha)*}(\{b|\mathbf{t}\}) \{b|\mathbf{t}\} \psi \\ &= \sum_b \sum_{\mathbf{R}_m} D_{ij}^{(\alpha)*}(\{b\}) \exp(i\mathbf{k} \cdot \mathbf{R}_m) \{b|\mathbf{t}\} \psi \end{aligned} \quad (8.6)$$

where the first summation is over all elements b of $G_0(k)$ and the second is over all primitive translations \mathbf{R}_m .

Now from equation (4.3) we have

$$\{b|\mathbf{t}\} = \{b|\mathbf{v}(b) + \mathbf{R}_m\} = \{b|\mathbf{v}(b)\} \{e|b^{-1}\mathbf{R}_m\} = \{b\} \{e|b^{-1}\mathbf{R}_m\} \quad (8.7)$$

and as \mathbf{R}_m runs over all primitive translations so does $\mathbf{R}_n = b^{-1}\mathbf{R}_m$, since the rotation b leaves the lattice of primitive translations invariant. Consequently, equation (8.6) may be written

$$\begin{aligned} \phi_{ij}^{(\alpha)} &= \sum_b \sum_{\mathbf{R}_n} D_{ij}^{(\alpha)*}(\{b\}) \{b\} \exp(i\mathbf{k} \cdot b\mathbf{R}_n) \{e|\mathbf{R}_n\} \psi \\ &= \sum_b \sum_{\mathbf{R}_n} D_{ij}^{(\alpha)*}(\{b\}) \{b\} \exp(ib^{-1}\mathbf{k} \cdot \mathbf{R}_n) \{e|\mathbf{R}_n\} \psi. \end{aligned} \quad (8.8)$$

But, since b (and hence b^{-1}) is an element of $G_0(k)$

$$\exp(ib^{-1}\mathbf{k}\cdot\mathbf{R}_n) = \exp(\mathbf{i}\mathbf{k}\cdot\mathbf{R}_n),$$

so that

$$\begin{aligned}\phi_{ij}^{(\alpha)} &= \sum_b \sum_{\mathbf{R}_n} D_{ij}^{(\alpha)*}(\{b\}) \{b\} \exp(\mathbf{i}\mathbf{k}\cdot\mathbf{R}_n) \{e|\mathbf{R}_n\} \psi \\ &= \sum_b D_{ij}^{(\alpha)*}(\{b\}) \{b\} \left(\sum_{\mathbf{R}_n} \exp(\mathbf{i}\mathbf{k}\cdot\mathbf{R}_n) \{e|\mathbf{R}_n\} \psi \right).\end{aligned}\quad (8\cdot9)$$

The sum over \mathbf{R}_n in equation (8·9) is now independent of b . From equations (5·3) and (8·3) we see that this sum gives a basis function $\phi_{\mathbf{k}}(\mathbf{x})$ for a one-dimensional representation of the subgroup \mathcal{T} of pure translations. Using the explicit form of equation (8·1), for the case $a = e$, we can express $\phi_{\mathbf{k}}(\mathbf{x})$ as a simple Bloch function,

$$\phi_{\mathbf{k}}(\mathbf{x}) = \sum_{\mathbf{R}_n} \exp(\mathbf{i}\mathbf{k}\cdot\mathbf{R}_n) \psi(\mathbf{x} - \mathbf{R}_n). \quad (8\cdot10)$$

Hence equation (8·6) finally reduces to

$$\phi_{ij}^{(\alpha)} = \sum_b D_{ij}^{(\alpha)*}(\{b\}) \{b\} \phi_{\mathbf{k}}. \quad (8\cdot11)$$

We note that the linear operator $\mathcal{L}_{\{b\}}$, which appears in abbreviated form in equation (8·11), involves the element $\{b\} = \{b|\mathbf{v}(b)\}$ of the reduced set $\{G_0(k)\}$; $\{b\}$ is not, in general, an element of the point group $G_0(k)$.

Koster (1957) shows that a basis function for an irreducible representation of \mathcal{X} in standard form, such as (8·11), is also a basis function for an irreducible representation of the entire space group G .

Equation (8·11) shows that one may construct basis functions without extending the ray representations of $G_0(k)$ to representations of \mathcal{X} and G via theorems 4 and 2. Provided one works always with Bloch functions, or other functions which transform irreducibly under \mathcal{T} (plane waves, orthogonalized plane waves, augmented plane waves, etc.), the matrices of the ray representations themselves suffice to project out basis functions for any desired irreducible representation. Furthermore, the matrix elements of these ray representations satisfy orthogonality relations (equation (2·2)) of precisely the same form as those for ordinary vector representations; these orthogonality relations may be used in the usual way to simplify secular equations, derive selection rules and so on.

Basis functions for the double space groups may be obtained in a very similar way; one need only replace equation (8·1) with equation (8·2), where g is now a two-component spinor function of position. Again, if Bloch functions are used throughout, one needs only the matrix elements of the appropriate ray representation of the point group $G_0(k)$. The factor system of this ray representation is given by combining minus signs from table 1 (or 2) with equation (6·4).

9. EXAMPLES

In order to use the matrix elements tabulated in the appendix one must first identify the factor system (6·4) with one appearing explicitly in tables A 0 to A 11. In some cases a gauge transformation of the form (2·6), (2·7) is required.

For space groups of low symmetry, that is when G_0 contains only a few elements, this identification is very easily made for all \mathbf{k} vectors on the surface of the Brillouin zone. Again for space groups of high symmetry the identification is very simple for \mathbf{k} vectors such that $G_0(k)$ contains only a few elements. The most complex cases are those where $G_0(k)$ contains

a large number of elements; up to 24 for space groups of the hexagonal system and up to 48 for those of the regular (cubic) system. Even here the calculations required to make the identifications are quite short, since initially we can concentrate on the generators of $G_0(k)$. Tables A 0 to A 11 show that never more than five generators are required.

In making the identifications we first work out the algebra of those elements $\{a\}, \{b\} \dots$ of the reduced set $\{G_0(k)\}$ which correspond to the generators a, b, \dots of the point group $G_0(k)$ using equation (6.4).[†] These elements $\{a\}, \{b\}, \dots$ will be referred to as the generators of $\{G_0(k)\}$. This algebra is then identified with one appearing explicitly in tables A 0 to A 11 for A, B, \dots , using a gauge transformation if necessary. Once the generators have been identified in this way the identification is extended to all elements of $\{G_0(k)\}$ by evaluating the products which label the matrices in tables A 1 to A 11.

We illustrate the procedure for several points of high symmetry in the regular holohedric space groups $O_h^1 \dots O_h^{10}$. These are, in fact, the most complex cases which arise for any space group.

Sets of generators for the groups $O_h^1 \dots O_h^{10}$ are given in table 3.

TABLE 3. GENERATORS OF THE REGULAR HOLOHEDRIC SPACE GROUPS $O_h^1 \dots O_h^{10}$

group	lattice [†]	generators of O_h and their non-primitive translations [‡]				
		$a = a_2$	$b = a_3$	$c = a_5$	$d = a_{23}$	$i = a'_1$
$O_h^1, Pm\bar{3}m$	Γ_r	0	0	0	0	0
$O_h^2, Pn\bar{3}n$	Γ_r	0	0	0	0	τ
$O_h^3, Pm\bar{3}n$	Γ_r	0	0	0	τ	0
$O_h^4, Pn\bar{3}m$	Γ_r	0	0	0	τ	τ
$O_h^5, Fm\bar{3}m$	Γ_r'	0	0	0	0	0
$O_h^6, Fm\bar{3}c$	Γ_r'	0	0	0	0	τ
$O_h^7, Fd\bar{3}m$	Γ_r'	0	0	0	τ	τ
$O_h^8, Fd\bar{3}c$	Γ_r'	0	0	0	τ_1	$-\tau_1$
$O_h^9, Im\bar{3}m$	Γ_r''	0	0	0	0	0
$O_h^{10}, Ia\bar{3}d$	Γ_r''	τ_1	τ_2	0	τ_7	0

$$\dagger \Gamma_r: \begin{aligned} \mathbf{t}_1 &= a\mathbf{i}, \\ \mathbf{t}_2 &= a\mathbf{j}, \\ \mathbf{t}_3 &= a\mathbf{k}. \end{aligned}$$

$$\Gamma_r': \begin{aligned} \mathbf{t}_1 &= \frac{1}{2}a(\mathbf{j} + \mathbf{k}), \\ \mathbf{t}_2 &= \frac{1}{2}a(\mathbf{k} + \mathbf{i}), \\ \mathbf{t}_3 &= \frac{1}{2}a(\mathbf{i} + \mathbf{j}). \end{aligned}$$

$$\Gamma_r'': \begin{aligned} \mathbf{t}_1 &= \frac{1}{2}a(-\mathbf{i} + \mathbf{j} + \mathbf{k}), \\ \mathbf{t}_2 &= \frac{1}{2}a(\mathbf{i} - \mathbf{j} + \mathbf{k}), \\ \mathbf{t}_3 &= \frac{1}{2}a(\mathbf{i} + \mathbf{j} - \mathbf{k}). \end{aligned}$$

$$\ddagger \text{ For } O_h^2, O_h^3, O_h^4; \tau = \frac{1}{2}a(\mathbf{i} + \mathbf{j} + \mathbf{k}) = \frac{1}{2}(\mathbf{t}_1 + \mathbf{t}_2 + \mathbf{t}_3).$$

$$\text{For } O_h^6; \tau = \frac{1}{2}a\mathbf{k} = \frac{1}{2}(\mathbf{t}_1 + \mathbf{t}_2 - \mathbf{t}_3).$$

$$\text{For } O_h^7; \tau = \frac{1}{4}a(\mathbf{i} + \mathbf{j} + \mathbf{k}) = \frac{1}{4}(\mathbf{t}_1 + \mathbf{t}_2 + \mathbf{t}_3).$$

$$\text{For } O_h^8; \tau_1 = \frac{1}{4}a(\mathbf{i} + \mathbf{j} + \mathbf{k}) = \frac{1}{4}(\mathbf{t}_1 + \mathbf{t}_2 + \mathbf{t}_3).$$

$$\text{For } O_h^{10}; \tau_1 = \frac{1}{2}a\mathbf{k} = \frac{1}{2}(\mathbf{t}_1 + \mathbf{t}_2), \tau_2 = \frac{1}{2}a\mathbf{i} = \frac{1}{2}(\mathbf{t}_2 + \mathbf{t}_3), \tau_7 = \frac{1}{4}a(\mathbf{i} + \mathbf{j} + \mathbf{k}) = \frac{1}{2}(\mathbf{t}_1 + \mathbf{t}_2 + \mathbf{t}_3).$$

The lattice Γ_r for $O_h^1 \dots O_h^4$ is the simple cubic lattice; the reciprocal lattice is also simple cubic with the Brillouin zone given in figure 3. From equation (5.1)

$$\mathbf{b}_1 = \frac{2\pi}{a}\mathbf{i}, \quad \mathbf{b}_2 = \frac{2\pi}{a}\mathbf{j}, \quad \mathbf{b}_3 = \frac{2\pi}{a}\mathbf{k}.$$

[†] Strictly, the algebra obtained from equation (6.4) applies not to the elements $\{b_i\} = \{b_i | \mathbf{v}(b_i)\}$ of $\{G_0(k)\}$ themselves but to the matrices $D(\{b_i\})$ which represent them in a ray representation of $G_0(k)$. However, for a given \mathbf{k} vector, the same algebra is obtained for all ray representations, so that it is legitimate and convenient to use this algebra also for the elements $\{b_i\}$ themselves.

The lattice Γ'_r for $O_h^5 \dots O_h^8$ is face-centred cubic; the reciprocal lattice is body centred cubic (figure 4).

$$\mathbf{b}_1 = \frac{2\pi}{a}(-\mathbf{i} + \mathbf{j} + \mathbf{k}), \quad \mathbf{b}_2 = \frac{2\pi}{a}(\mathbf{i} - \mathbf{j} + \mathbf{k}), \quad \mathbf{b}_3 = \frac{2\pi}{a}(\mathbf{i} + \mathbf{j} - \mathbf{k}).$$

Finally, O_h^9 and O_h^{10} have the body-centred lattice Γ''_r ; their reciprocal lattice is face-centred cubic with the Brillouin zone shown in figure 5.

$$\mathbf{b}_1 = \frac{2\pi}{a}(\mathbf{k} + \mathbf{j}), \quad \mathbf{b}_2 = \frac{2\pi}{a}(\mathbf{k} + \mathbf{i}), \quad \mathbf{b}_3 = \frac{2\pi}{a}(\mathbf{i} + \mathbf{j}).$$

The labelling of the special points in figures 3 to 5 follows Koster (1957).

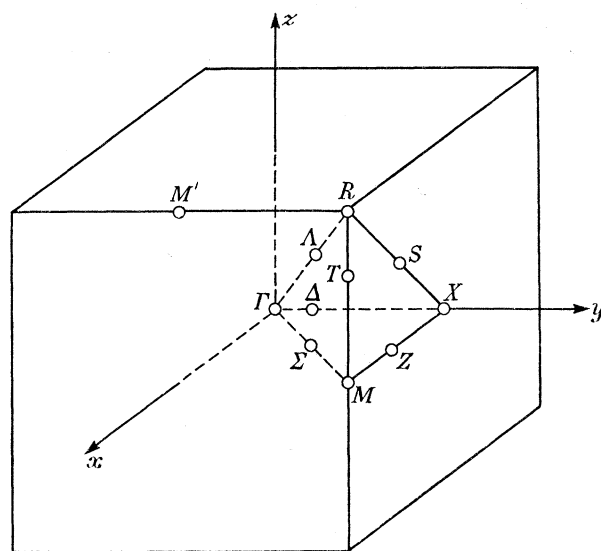


FIGURE 3. Brillouin zone for the space groups $O_h^1 \dots O_h^4$.

From table 3 we see that the groups O_h^1 , O_h^5 and O_h^9 are symmorphich. For these groups the representations of \mathcal{K} are given by equation (6.7) and the tables of McWeeny (1963) for \mathbf{k} vectors either within or on the surface of the Brillouin zone. However, the additional representations of the double groups \mathcal{K}_d will be obtained by the method of ray representations, since explicit matrices are not available in the literature for the additional representations of the double point groups.†

The points of high symmetry which we shall consider are:

(i) The points Γ and R for $O_h^1 \dots O_h^4$; Γ and H for O_h^9 and O_h^{10} . If, in figures 3 and 5, we mark in all points equivalent to R and H , we see that for these points, as for Γ , \mathcal{K} is the full space group and the point group $G_0(k)$ is O_h . For $O_h^5 \dots O_h^8$ there is no point other than Γ which displays the full symmetry O_h .

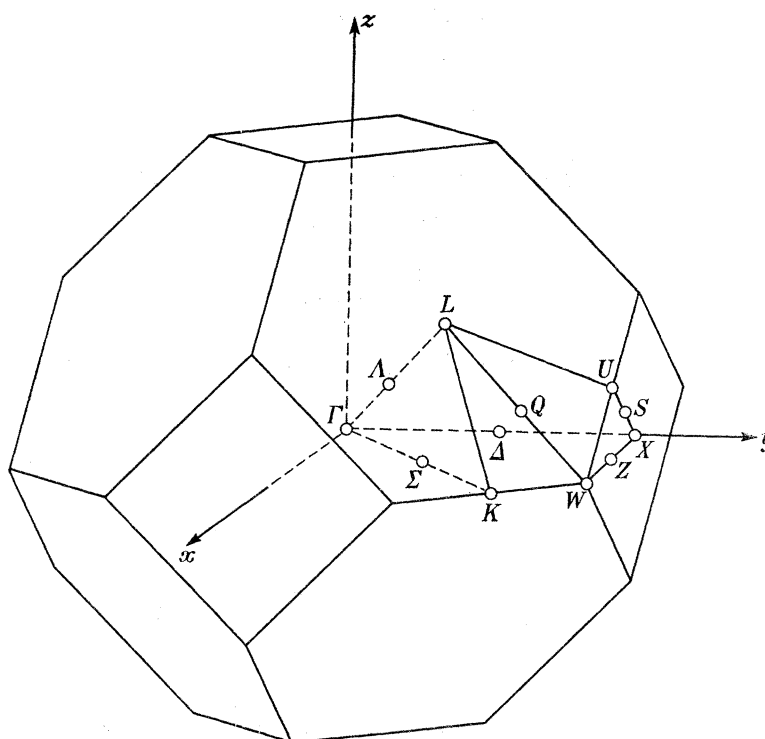
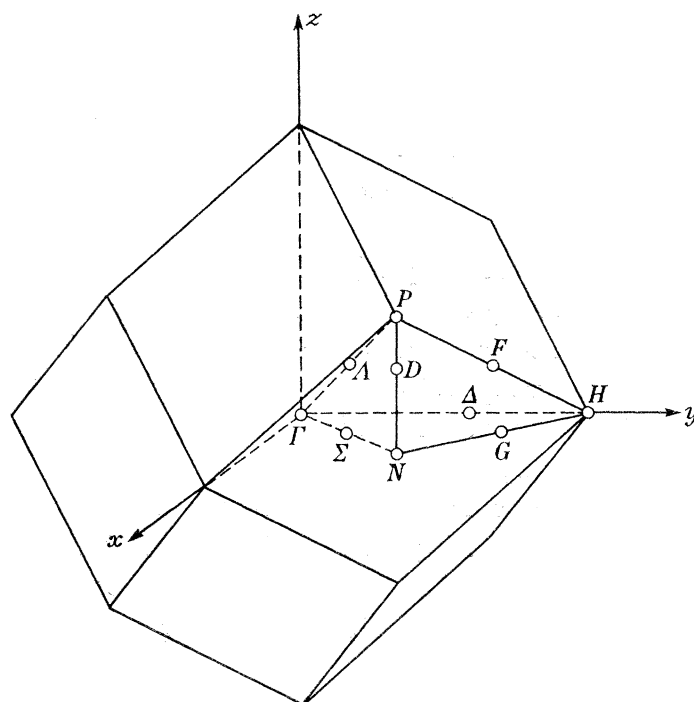
(ii) The point P for O_h^9 and O_h^{10} ; $G_0(k) = T_d$,

(iii) The point X for $O_h^1 \dots O_h^8$; $G_0(k) = D_{4h}$,

(iv) The point L for $O_h^5 \dots O_h^8$; $G_0(k) = D_{3d}$,

(v) The point M for $O_h^1 \dots O_h^4$; $G_0(k) = D_{4h}$.

† These matrices may alternatively be generated from the basis functions listed by Koster, Dimmock, Wheeler & Statz (1963); see also Kovalev (1961).

FIGURE 4. Brillouin zone for the space groups $O_h^5 \dots O_h^8$.FIGURE 5. Brillouin zone for the space groups $O_h^9 \dots O_h^{10}$.

The explicit identifications for these points, which include all those for which the order of $G_0(k)$ is greater than 8, are given in tables 4 to 7. The identifications for the spin representations are simply the product of the factor for the representation without spin and the factor for the spin representation of the point group.

TABLE 4. MINIMAL NON-PRIMITIVE TRANSLATIONS OF SPACE GROUPS O_h^n . IDENTIFICATIONS AT R , H AND P , AND FOR SPIN REPRESENTATIONS OF $O_h(O_h^s)$

label (tables A9, A11)		minimal non-primitive translations†							identifications							
		O_h^2	O_h^3	O_h^4	O_h^6	O_h^7	O_h^8	O_h^{10}	$O_h^1 - O_h^{10}$ Γ		O_h^2 R	O_h^3 R	O_h^4 R	O_h^{10} H	O_h^{10} P ‡	O_h^s T_d^s
									α	β						
	O_h															
<i>E</i>	a_1	1	1	1	1	1	1	1	1
<i>A</i>	a_2	τ_1	1	1	1	1	-1	i	1	1
<i>B</i>	a_3	τ_2	1	1	1	1	-1	i	1	1
<i>AB</i>	a_4	τ_3	1	1	1	1	-1	i	1	1
<i>C</i>	a_5	1	1	1	1	1	1	1	-1
<i>C²</i>	a_9	1	1	1	1	1	1	1	-1
<i>AC</i>	a_7	τ_1	1	1	1	1	-1	i	1	1
<i>BC</i>	a_8	τ_2	1	1	1	1	-1	i	1	1
<i>ABC</i>	a_6	τ_3	1	1	1	1	-1	i	1	1
<i>AC²</i>	a_{12}	τ_1	1	1	1	1	-1	i	-1	-1
<i>BC²</i>	a_{10}	τ_2	1	1	1	1	-1	i	-1	-1
<i>ABC²</i>	a_{11}	τ_3	1	1	1	1	-1	i	-1	-1
<i>D</i>	a_{23}	.	τ	τ	.	τ	τ_1	τ_7	1	1	1	1	1	s'	i	i
<i>CD</i>	a_{21}	.	τ	τ	.	τ	τ_1	τ_7	1	1	1	1	1	s'	i	i
<i>C²D</i>	a_{19}	.	τ	τ	.	τ	τ_1	τ_7	1	1	1	1	-1	s'	-i	-i
<i>AD</i>	a_{18}	.	τ	τ	.	τ	τ_1	τ_5	1	1	1	1	-1	r'	-i	-i
<i>ABCD</i>	a_{16}	.	τ	τ	.	τ	τ_1	τ_4	1	1	1	1	-1	r'	-i	-i
<i>BC²D</i>	a_{14}	.	τ	τ	.	τ	τ_1	τ_6	1	1	1	1	-1	r'	-i	-i
<i>BD</i>	a_{17}	.	τ	τ	.	τ	τ_1	τ_6	1	1	1	1	-1	r'	i	i
<i>ACD</i>	a_{15}	.	τ	τ	.	τ	τ_1	τ_5	1	1	1	1	-1	r'	i	i
<i>ABC²D</i>	a_{13}	.	τ	τ	.	τ	τ_1	τ_4	1	1	1	1	-1	r'	i	i
<i>ABD</i>	a_{24}	.	τ	τ	.	τ	τ_1	τ_4	1	1	1	1	-1	r'	i	i
<i>BCD</i>	a_{22}	.	τ	τ	.	τ	τ_1	τ_6	1	1	1	1	-1	r'	i	i
<i>AC²D</i>	a_{20}	.	τ	τ	.	τ	τ_1	τ_5	1	1	1	1	-1	r'	i	i
<i>I</i>	a'_1	τ	.	τ	τ	τ	$-\tau_1$.	1	1	1	1	1	.	1	1
<i>AI</i>	a'_2	τ	.	τ	τ	τ	$-\tau_1$	τ_1	1	1	1	1	-1	.	1	1
<i>BI</i>	a'_3	τ	.	τ	τ	τ	$-\tau_1$	τ_2	1	1	1	1	-1	.	1	1
<i>ABI</i>	a'_4	τ	.	τ	τ	τ	$-\tau_1$	τ_3	1	1	1	1	-1	.	1	1
<i>CI</i>	a'_5	τ	.	τ	τ	τ	$-\tau_1$.	1	1	1	1	1	.	-1	-1
<i>C²I</i>	a'_9	τ	.	τ	τ	τ	$-\tau_1$.	1	1	1	1	1	.	-1	-1
<i>ACI</i>	a'_7	τ	.	τ	τ	τ	$-\tau_1$	τ_1	1	1	1	1	-1	.	1	1
<i>BCI</i>	a'_8	τ	.	τ	τ	τ	$-\tau_1$	τ_2	1	1	1	1	-1	.	1	1
<i>ABCI</i>	a'_6	τ	.	τ	τ	τ	$-\tau_1$	τ_3	1	1	1	1	-1	.	1	1
<i>AC²I</i>	a'_{12}	τ	.	τ	τ	τ	$-\tau_1$	τ_1	1	1	1	1	-1	.	-1	-1
<i>BC²I</i>	a'_{10}	τ	.	τ	τ	τ	$-\tau_1$	τ_2	1	1	1	1	-1	.	-1	-1
<i>ABC²I</i>	a'_{11}	τ	.	τ	τ	τ	$-\tau_1$	τ_3	1	1	1	1	-1	.	-1	-1
<i>DI</i>	a'_{23}	τ	τ	.	τ	.	τ_2	τ_7	1	-1	1	1	1	.	i	i
<i>CDI</i>	a'_{21}	τ	τ	.	τ	.	τ_2	τ_7	1	-1	1	1	1	.	i	i
<i>C²DI</i>	a'_{19}	τ	τ	.	τ	.	τ_2	τ_7	1	-1	1	1	1	.	i	i
<i>ADI</i>	a'_{18}	τ	τ	.	τ	.	τ_2	τ_5	1	-1	1	1	-1	.	-i	-i
<i>ABCDI</i>	a'_{16}	τ	τ	.	τ	.	τ_2	τ_4	1	-1	1	1	-1	.	-i	-i
<i>BC²DI</i>	a'_{14}	τ	τ	.	τ	.	τ_2	τ_6	1	-1	1	1	-1	.	-i	-i
<i>BDI</i>	a'_{17}	τ	τ	.	τ	.	τ_2	τ_6	1	-1	1	1	-1	.	i	i
<i>ACDI</i>	a'_{15}	τ	τ	.	τ	.	τ_2	τ_5	1	-1	1	1	-1	.	i	i
<i>ABC²DI</i>	a'_{13}	τ	τ	.	τ	.	τ_2	τ_4	1	-1	1	1	-1	.	i	i
<i>ABDI</i>	a'_{24}	τ	τ	.	τ	.	τ_2	τ_4	1	-1	1	1	-1	.	i	i
<i>BCDI</i>	a'_{22}	τ	τ	.	τ	.	τ_2	τ_6	1	-1	1	1	-1	.	i	i
<i>AC²DI</i>	a'_{20}	τ	τ	.	τ	.	τ_2	τ_5	1	-1	1	1	-1	.	i	i

† See footnotes to table 3. In addition: for O_h^8 ; $\tau_2 = \frac{1}{2}ak = \frac{1}{2}(t_1 + t_2 - t_3)$. For O_h^{10} ; $\tau_3 = \frac{1}{2}aj = \frac{1}{2}(t_1 + t_3)$, $\tau_4 = \frac{1}{4}a(-i + j + k) = \frac{1}{2}t_1$, $\tau_5 = \frac{1}{4}a(i - j + k) = \frac{1}{2}t_2$, $\tau_6 = \frac{1}{4}a(i + j - k) = \frac{1}{2}t_3$.

‡ At P , $G_0(k) = T_d$, $d = a'_{23}$ (table A 9) and elements a_{23} , a_{21} , ..., a_{20} appear dashed in $G_0(k)$ and \mathcal{K} . e.g. $ABCD = r\{a'_{16}|\tau_4\}$. $r = (1+i)/\sqrt{2}$, $s = (1-i)/\sqrt{2}$.

§ For O_h^8 only.

TABLE 5. IDENTIFICATIONS AT POINTS X AND M' , AND FOR SPIN REPRESENTATIONS OF $D_{4h}(D_{4h}^s)$

label (table A 8)	O_h^2 X	O_h^2 $M' \dagger$	O_h^3 X	O_h^3 M'	O_h^4 X	O_h^4 M'	O_h^6 X	O_h^7 X	O_h^8 X	D_{4h}^s
α	1	1	1	1	1	1	1	1	1	-1
β	1	-1	-1	1	-1	-1	1	-1	-1	1
γ	-1	-1	1	1	-1	-1	1	-1	-1	-1
$D_{4h} \ddagger$										
E	a_1	1	1	1	1	1	1	1	1	1
A	a_{16}	1	i	i	1	i	1	i	i	i
A^2	a_3	1	-1	1	-1	1	1	1	1	-1
A^3	a_{15}	1	-i	i	-1	i	1	i	i	i
B	a'_2	i	i	1	1	i	1	i	i	i
AB	a'_{21}	i	1	i	1	1	1	1	-1	1
A^2B	a'_4	i	-i	1	-1	i	1	i	i	i
A^3B	a'_{22}	i	-1	i	-1	1	1	1	-1	-1
C	a'_3	1	1	1	1	1	1	1	1	i
AC	a'_{15}	1	-i	i	1	-i	1	-i	i	1
A^2C	a'_1	1	-1	1	-1	1	1	1	1	i
A^3C	a'_{16}	1	i	i	-1	-i	1	-i	i	-1
BC	a_4	-i	-i	1	1	-i	1	-i	-i	-1
ABC	a_{22}	-i	1	i	1	1	1	1	1	-i
A^2BC	a_2	-i	i	1	-1	-i	1	-i	-i	1
A^3BC	a_{21}	-i	-1	i	-1	1	1	1	1	-i

† To facilitate tabulation M' , where $G_0(k)$ is the same as at X , is considered here in place of M (figure 3). For identifications at M we use the isomorphism $\{a_{16}\} \leftrightarrow \{a_{18}\}$, $\{a_2\} \leftrightarrow \{a'_3\}$, $\{a_3\} \leftrightarrow \{a'_4\}$, etc.

‡ Non-primitive translations of elements of reduced set $\{G_0(k)\} = \{D_{4h}\}$ appear in table 4.

TABLE 6. IDENTIFICATIONS AT THE POINT L , AND FOR SPIN REPRESENTATIONS OF $D_{3d}(D_{3d}^s)$

label (table A 5)	O_h^6	O_h^7	O_h^8	D_{3d}^s
α	-1	1	-1	1
$D_{3d} \ddagger$				
E	a_1	1	1	1
A	a'_5	1	1	1
A^2	a_9	1	1	-1
A^3	a'_1	1	1	-1
A^4	a_5	1	1	-1
A^5	a'_9	1	1	1
B	a'_{23}	i	1	i
AB	a_{21}	i	1	-i
A^2B	a'_{19}	i	1	i
A^3B	a_{23}	i	1	-i
A^4B	a_{21}	i	1	i
A^5B	a'_{19}	i	1	-i

† Non-primitive translations of elements of reduced set $\{G_0(k)\} = \{D_{3d}\}$ appear in table 4.

Also shown in table 4 are the minimal non-primitive translations appearing in the elements of the reduced set $\{G_0\}$ for the non-symmorphic groups O_h^n . These may be obtained by forming appropriate products of the generators of table 3 or directly from the *International tables* (1953). The ordering of the elements in tables 4 to 7 is chosen to agree with that in the tables of the appendix.

Five fully worked examples will illustrate the methods used to derive the results of tables 4 to 7. Similar calculations will yield the identifications for any \mathbf{k} vector and any space group.

Example 1

O_h^2 at the point R , $\mathbf{k} = (\pi/a) (\mathbf{i} + \mathbf{j} + \mathbf{k}) = \frac{1}{2}(\mathbf{b}_1 + \mathbf{b}_2 + \mathbf{b}_3)$.

Here \mathcal{H} is the full space group. The generators of the reduced set $\{G_0(k)\}$ are, from table 3,

$$\{a\} = \{a_2 | 0\}, \quad \{b\} = \{a_3 | 0\}, \quad \{c\} = \{a_5 | 0\}, \quad \{d\} = \{a_{23} | 0\}, \quad \{i\} = \{a'_1 | \frac{1}{2}a(\mathbf{i} + \mathbf{j} + \mathbf{k})\}.$$

Since $\{a\}$, $\{b\}$, $\{c\}$ and $\{d\}$ have zero non-primitive translations they satisfy the point group algebra given at the head of table A 11 for a , b , c and d . We, therefore, immediately make the identifications

$$A = \{a\}, \quad B = \{b\}, \quad C = \{c\}, \quad D = \{d\}, \quad \alpha = 1. \quad (9.1)$$

Products involving $\{i\}$ are, however, affected by the non-primitive translation $\boldsymbol{\tau} = \frac{1}{2}a(\mathbf{i} + \mathbf{j} + \mathbf{k})$. Using equation (4.7), table 1 and figure 1 we find

$$\{i\}^2 = \{a'_1 | \boldsymbol{\tau}\} \{a'_1 | \boldsymbol{\tau}\} = \{a_1 | a'_1 \boldsymbol{\tau} + \boldsymbol{\tau}\} = \{a_1 | -\boldsymbol{\tau} + \boldsymbol{\tau}\} = \{e | 0\} = \{e\}.$$

Similarly,

$$\left. \begin{aligned} \{i\} \{a\} &= \{e | a(\mathbf{j} + \mathbf{k})\} \{a\} \{i\} = \{a\} \{i\}, \\ \{i\} \{b\} &= \{e | a(\mathbf{i} + \mathbf{k})\} \{b\} \{i\} = \{b\} \{i\}, \\ \{i\} \{c\} &= \{c\} \{i\}, \\ \{i\} \{d\} &= \{e | a(\mathbf{i} + \mathbf{j} + \mathbf{k})\} \{d\} \{i\} = -\{d\} \{i\}. \end{aligned} \right\} \quad (9.2)$$

Here the final expressions for the products are obtained from equation (6.4) with $\mathbf{k} = (\pi/a) (\mathbf{i} + \mathbf{j} + \mathbf{k})$ (see footnote on p. 19).

Comparing equation (9.2) with the algebra listed for A , B , C , D and I at the head of table A 11, we see that no gauge transformation is required and that the identification of the generators of $\{G_0(k)\}$ is completed by

$$I = \{i\}, \quad \beta = -1. \quad (9.3)$$

Finally, to obtain the complete identification shown in table 4, the products which label the matrices in table A 11 are evaluated by means of the identifications (9.1) and (9.3) and taking the non-primitive translation $\boldsymbol{\tau}$ into account.

For example

$$\begin{aligned} AI &= \{a\} \{i\} = \{a_2 | 0\} \{a'_1 | \boldsymbol{\tau}\} = \{a'_2 | a_2 \boldsymbol{\tau}\} = \{a_1 | a(-\mathbf{j} - \mathbf{k})\} \{a'_2 | \boldsymbol{\tau}\} \\ &= \{a'_2 | \boldsymbol{\tau}\} \end{aligned}$$

$$\begin{aligned} DI &= \{a_{23} | 0\} \{a'_1 | \boldsymbol{\tau}\} = \{a'_{23} | a_{23} \boldsymbol{\tau}\} = \{a_1 | a(-\mathbf{i} - \mathbf{j} - \mathbf{k})\} \{a'_{23} | \boldsymbol{\tau}\} \\ &= -\{a'_{23} | \boldsymbol{\tau}\}. \end{aligned}$$

Here again the final expressions are obtained from equation (6.4) with

$$\mathbf{k} = (\pi/a) (\mathbf{i} + \mathbf{j} + \mathbf{k}).$$

We note that the identification of each product of A, B, \dots is obtained by evaluating a single product of elements of $\{G_0(k)\}$. Allowing for the products needed to identify the generators (equation (9·2)), we see that rather more than g_k products are needed to obtain the complete identification, where g_k is the order of $G_0(k)$. Thus when g_k is large, far fewer products are required than the g_k^2 which would appear in a complete multiplication table. It is therefore simpler to evaluate each product directly from table 1 and figure 1 (or table 2 and figure 2). Of course in this example and, indeed, in most cases, many of the products are trivial because of the zero non-primitive translations associated with some elements.

However, if one wishes to check the results by projecting out basis functions (equation (8·11)) and operating on these functions with all the elements of $\{G_0(k)\}$ (Slater 1965), it is worthwhile constructing an explicit multiplication table. This procedure provides a very thorough check of the representation matrices.

Using the full identification shown in table 4, we obtain directly from table A 11 three representations; Γ_1 and Γ_2 of dimension 2, and Γ_3 of dimension 6. From the arbitrary factors ± 1 for D and I listed at the head of table A 11 we obtain one new representation Γ'_2 which differs from Γ_2 in that the sign of I is reversed throughout, that is the identifications (9·1) and (9·3) are replaced by

$$A = \{a\}, \quad B = \{b\}, \quad C = \{c\}, \quad D = \{d\}, \quad I = -\{i\}. \quad (9\cdot4)$$

Clearly this identification (9·4) is also consistent with the algebra listed for A, B, C, D, I with $\alpha = 1, \beta = -1$.

Changing the sign of D in Γ_2 , and the signs of D and/or I in Γ_1 and Γ_3 leads to no new representations, because the characters of these elements and their products all vanish. We merely obtain similarity transforms of representations obtained previously.

Hence, finally, we obtain three two-dimensional and one six-dimensional representation. Since $3 \times 2^2 + 6^2 = 48$ we know from equation (2·5) that this set of representations is complete.

The identifications for the spin representations of \mathcal{K} at the point R in O_h^2 could be found in a similar way by introducing appropriate minus signs from table 1 into equations (9·2) and the equations satisfied by a, b, c, d (table A 11). This is unnecessary, however, if the identifications for the spin representations of the point group O_h are available (table 4, final column). The factors in the identification at R in O_h^2 with spin are just the products of the factors without spin and the factors for the spin representations of O_h . The values of the parameters α and β , in this case $\alpha = -1, \beta = -1$, are obtained in the same way.

Referring to table A 11, $\alpha = -1, \beta = -1$ we find two four-dimensional representations Γ_1 and Γ_2 listed explicitly. A third four-dimensional representation Γ'_1 is obtained by reversing the sign of I in Γ_1 . Again equation (2·5) shows that this set of representations is complete ($3 \times 4^2 = 48$).

Example 2

O_h^7 at the point X ; $\mathbf{k} = (2\pi/a)\mathbf{j} = \frac{1}{2}(\mathbf{b}_1 + \mathbf{b}_3)$. From figure 4, $G_0(k) = D_{4h}$. From table A 8 the generators of $G_0(k)$ are

$$a = (4)_y = a_{16}, \quad b = m_{yz} = a'_2, \quad c = m_{xz} = a'_3.$$

From the *International tables* (1953) the generators of $\{G_0(k)\}$ are

$$\{a\} = \{a_{16} | \tau\}, \quad \{b\} = \{a'_2 | \tau\}, \quad \{c\} = \{a'_3 | \tau\} \quad \text{where } \tau = \frac{1}{4}a(\mathbf{i} + \mathbf{j} + \mathbf{k}).$$

The algebra of these generators of $\{G_0(k)\}$ is evaluated as in example 1, with the aid of table 1, figure 1 and equation (6.4). We find

$$\left. \begin{aligned} \{a\}^4 &= \{e\}, \\ \{b\}^2 &= -\{e\}, \quad \{b\}\{a\} = -\{a\}^3\{b\}, \\ \{c\}^2 &= \{e\}, \quad \{c\}\{a\} = -\{a\}\{c\}, \quad \{c\}\{b\} = -\{b\}\{c\}. \end{aligned} \right\} \quad (9.5)$$

Comparing the algebra (9.5) with those listed at the head of table A 8 for A , B and C , we see that the minus signs must be removed from the equations

$$\{b\}^2 = -\{e\}, \quad \{b\}\{a\} = -\{a\}^3\{b\}.$$

This is achieved, without spoiling the other relations, by the identifications

$$A = i\{a\}, \quad B = i\{b\}, \quad C = \{c\}. \quad (9.6)$$

From equations (9.5) and (9.6) we obtain the algebra

$$\left. \begin{aligned} A^4 &= E, \\ B^2 &= E, \quad BA = A^3B, \\ C^2 &= E, \quad CA = -AC, \quad CB = -BC, \end{aligned} \right\} \quad (9.7)$$

which agrees with the case $\alpha = 1$, $\beta = -1$, $\gamma = -1$ listed explicitly in table A 8. Equations (9.6) is an example of the gauge transformations that are sometimes necessary in identifying the generators. All other cases which arise are equally simple.

Again the complete identification given in table 5 is obtained by evaluating the products which label the matrix elements in table A 8.

From table A 8, $\alpha = 1$, $\beta = -1$, $\gamma = -1$ we obtain two two-dimensional representations Γ_1 and Γ_2 directly, and two others Γ'_1 and Γ'_2 by reversing the sign of B . These dimensionalities satisfy equation (2.5) ($4 \times 2^2 = 16$) showing that we have a complete set of representations.

The identification for the spin representations is given by the products of entries in columns 10 and 12 of table 5. We find $\alpha = -1$, $\beta = -1$, $\gamma = 1$ and (from table A 8) one four-dimensional representation ($4^2 = 16$).

Example 3

Spin representations of the point group D_{4h} . Here the factor system is obtained directly from the bars in table 1. We find that the generators

$$\{a\} = \{a_{16} | 0\}, \quad \{b\} = \{a'_2 | 0\}, \quad \{c\} = \{a'_3 | 0\}$$

of D_{4h} with spin (D_{4h}^s) satisfy the algebra†

$$\left. \begin{aligned} \{a\}^4 &= -\{e\}, \\ \{b\}^2 &= -\{e\}, \quad \{b\}\{a\} = -\{a\}^3\{b\}, \\ \{c\}^2 &= -\{e\}, \quad \{c\}\{a\} = \{a\}\{c\}, \quad \{c\}\{b\} = -\{b\}\{c\}. \end{aligned} \right\} \quad (9.8)$$

Comparing equations (9.8) with table A 8, we make the identifications

$$A = i\{a\}, \quad B = i\{b\}, \quad C = i\{c\},$$

† Since all translations are zero we might equally well write $a^4 = -e$, etc. The brackets are retained to emphasize the similarity with the other examples, and to avoid confusion with the algebra listed in table A 8 for a , b , c .

which give the algebra

$$\left. \begin{aligned} A^4 &= -E, & \alpha &= -1; \\ B^2 &= E, \quad BA = A^3B, & \beta &= 1; \\ C^2 &= E, \quad CA = AC, \quad CB = -BC, & \gamma &= -1. \end{aligned} \right\} \quad (9.9)$$

The full identification is shown in table 5. From table A 8, $\alpha = -1$, $\beta = 1$, $\gamma = -1$ we find one two-dimensional representation Γ_1 , directly. Three others Γ'_1 , Γ''_1 , Γ'''_1 are obtained by reversing the signs of A and/or C ($4 \times 2^2 = 16$).

These ray representations of D_{4h} may be extended to vector representations (the additional representations) of the double group $D_{4h,d}$ using equation (7.2).

Example 4

Spin representations of D_{3d} .

From table A 5, figure 1, and table 1 (figure 2 and table 2 could also be used in this case), we obtain the generators of D_{3d}^s

$$\{a\} = \{a'_5 | 0\}, \quad \{b\} = \{a'_{23} | 0\},$$

with the algebra

$$\{a\}^6 = \{e\},$$

$$\{b\}^2 = -\{e\}, \quad \{b\}\{a\} = \{a\}^5\{b\}.$$

After making the identifications $A = \{a\}$, $B = i\{b\}$,

we obtain the usual algebra of the point group D_{3d}

$$A^6 = E, \quad B^2 = E, \quad BA = A^5B.$$

The identification is completed (table 6) by evaluating the products which label the matrices in table A 5. However, in a case such as this where we find the normal point group algebra, that is a vector representation, the representation matrices are obtained not from table A 5 but from the appropriate table of McWeeny (1963) (namely, his table (4.9), p. 98). The expressions for the elements of tables 1 and 2 in McWeeny's notation is evident from figures 1 and 2.

When $G_0(k)$ is one of the point groups C_1 , C_i , C_2 , C_s , C_3 , S_4 , C_4 , C_6 , C_{3i} , D_3 , C_{3v} , C_{3h} not appearing explicitly in tables A 1 to A 11, we necessarily have the situation encountered here; a gauge transformation associates the algebra of the generators of $\{G_0(k)\}$ with the usual point-group algebra, and, apart from the gauge transformation we have ordinary vector representations. All the above-mentioned point groups are cyclic, with the trivial algebra $a^n = e$, except for the isomorphic pair D_3 and C_{3v} . The geometrical identification and algebra of the generators of these two groups are given in table A 0. Although these groups have no non-trivial ray representations, this algebra is useful in determining the appropriate gauge transformations.

Example 5

$$O_h^{10} \text{ at the point } H; \mathbf{k} = (2\pi/a) \mathbf{j} = \frac{1}{2}(\mathbf{b}_1 - \mathbf{b}_2 + \mathbf{b}_3)$$

$$G_0(k) = O_h.$$

From table 3 the generators of $\{G_0(k)\}$ are

$$\{a\} = \{a_2 | \frac{1}{2}a(\mathbf{k})\}, \quad \{b\} = \{a_3 | \frac{1}{2}a(\mathbf{i})\}, \quad \{c\} = \{a_5 | 0\}, \quad \{d\} = \{a_{23} | \frac{1}{4}a(\mathbf{i} + \mathbf{j} + \mathbf{k})\}, \quad \{\mathbf{i}\} = \{a'_1 | 0\},$$

whose algebra is found to be (table 1, figure 1, equation (6·4))

$$\left. \begin{aligned} \{a\}^2 &= \{e\}; \\ \{b\}^2 &= \{e\}, \quad \{b\}\{a\} = \{a\}\{b\}; \\ \{c\}^3 &= \{e\}, \quad \{c\}\{a\} = \{b\}\{c\}, \quad \{c\}\{b\} = -\{a\}\{b\}\{c\}; \\ \{d\}^2 &= \{e\}, \quad \{d\}\{a\} = \{b\}\{d\}, \quad \{d\}\{b\} = \{a\}\{d\}, \quad \{d\}\{c\} = \{c\}^2\{d\}; \\ \{i\}^2 &= \{e\}, \quad \{i\}\{a\} = \{a\}\{i\}, \quad \{i\}\{b\} = \{b\}\{i\}, \quad \{i\}\{c\} = \{c\}\{i\}, \quad \{i\}\{d\} = -\{d\}\{i\} \end{aligned} \right\} (9\cdot10)$$

Comparing equations (9·10) with table A 11 we make the identifications

$$A = -\{a\}, \quad B = -\{b\}, \quad C = \{c\}, \quad D = \{d\}, \quad I = \{i\}; \quad \alpha = 1, \quad \beta = -1.$$

The full identifications, with and without spin, are given in table 4. Without spin, we find three two-dimensional representations Γ_1 , Γ_2 , Γ'_2 and one six-dimensional representation Γ_3 ; with spin $\alpha = -1$, $\beta = -1$ and there are three four-dimensional representations Γ_1 , Γ'_1 and Γ_2 .

This final example is one of the most complex cases which arise for any space group. Even here the identifications, both with and without spin, appear as the result of quite brief calculations.

10. TIME REVERSAL, COMPATIBILITY RELATIONS AND SPIN ORBIT SPLITTING

In addition to the degeneracies which arise from spatial symmetry further degeneracies may be produced by the invariance of the Hamiltonian under time reversal. These degeneracies may also be determined from the ray representations both without and with spin. Since this subject is fully covered in Koster's (1957) review article, we will not discuss it further, except to mention that for the determination of time reversal degeneracies the characters of the representations are sufficient; one does not need the full matrices.

The characters are also sufficient to determine the compatibility relations between representations at neighbouring points in the Brillouin zone and the splitting of bands under the action of spin orbit coupling. If the latter problem is treated directly in terms of ray representations, without invoking the double groups, attention must be paid to changes in the factor system when Kronecker products are formed. (Cf. § 2.)

For example, the Kronecker product of the ray representation $\alpha = 1$, $\beta = -1$, Γ_3 of O_h with the standard spin representation of O_h , $\alpha = -1$, $\beta = 1$, Γ_1 gives a ray representation with $\alpha = -1$, $\beta = -1$. Since, in this case, the character of the Kronecker product is (from table A 11)

$$\chi(E) = 12 \quad \text{all others zero,}$$

we find from table A 11 $\alpha = -1$, $\beta = -1$ the reduction

$$\begin{aligned} \Gamma_3(\alpha = 1, \beta = -1) \\ \times \Gamma_1(\alpha = -1, \beta = 1) &= \Gamma_1(\alpha = -1, \beta = -1) + \Gamma'_1(\alpha = -1, \beta = -1), \\ &+ \Gamma_2(\alpha = -1, \beta = -1). \end{aligned} \quad (10\cdot1)$$

In equation (10·1) $\Gamma'_1(\alpha = -1, \beta = -1)$ is the representation obtained from the listed representation $\Gamma_1(\alpha = -1, \beta = -1)$ by reversing the sign of I throughout.

Equation (10·1) gives the splitting under spin-orbit coupling of the sixfold degenerate state at the point R in O_h^3 (table 4). The spin orbit coupling splits the original $6 \times 2 = 12$ -fold degeneracy into three fourfold degenerate states.

11. SLATER'S CONVENTIONS

Slater (1965) has recently derived matrices for the irreducible representations of a number of space groups using a set of conventions which agree with those used here and by Koster (1957) except at one point. In Slater's work equation (8.1) is replaced by the equation

$$L_{\{a|\mathbf{t}\}}f(\mathbf{x}) = f(\{a|\mathbf{t}\}\mathbf{x}). \quad (11.1)$$

The natural mapping

$$L_{\{a|\mathbf{t}\}} \leftrightarrow \{a|\mathbf{t}\} \quad (11.2)$$

no longer provides an isomorphism between the group G_L of linear operators $L_{\{a|\mathbf{t}\}}$ and the space group G with elements $\{a|\mathbf{t}\}$, as was the case in § 8. This causes no difficulty in Slater's work since he deals throughout with the group G_L rather than with the space group G ; for example the product rule is derived, not by transforming a general vector \mathbf{x} with $\{b|\mathbf{s}\}$, $\{a|\mathbf{t}\}$ (cf. § 4), but by operating successively with $L_{\{b|\mathbf{s}\}}$, $L_{\{a|\mathbf{t}\}}$ on a general function $f(\mathbf{x})$. Consequently, in the Slater theory, equation (4.3) is replaced by

$$L_{\{a|\mathbf{t}\}}L_{\{b|\mathbf{s}\}} = L_{\{ba|b\mathbf{t}+\mathbf{s}\}}. \quad (11.3)$$

Again Slater's 'multiplication table for successive operations on a plane wave', which corresponds to the factor system (6.4) of a ray representation, is obtained by operating successively with $L_{\{b|\mathbf{s}\}}$, $L_{\{a|\mathbf{t}\}}$ on a plane wave

$$f(\mathbf{x}) = \exp(i(\mathbf{k} + \mathbf{K}_n) \cdot \mathbf{x}). \quad (11.4)$$

Since Slater's work is fully described elsewhere (Slater 1965) we shall not consider it further except to point out the obvious relation between his representation matrices and those obtained here. To describe this relationship we introduce groups \mathcal{T}_L , \mathcal{K}_L , G_{0L} , $G_{0L}(k)$ which are related to \mathcal{T} , \mathcal{K} , G_0 and $G_0(k)$ in the same way as G_L is related to G .

The mapping

$$L_{\{a|\mathbf{t}\}} \leftrightarrow \{a|\mathbf{t}\}^{-1} \quad (11.5)$$

now provides the isomorphisms

$$G_L \cong G, \quad \mathcal{T}_L \cong \mathcal{T}, \quad \mathcal{K}_L \cong \mathcal{K}, \quad G_{0L} \cong G_0, \quad G_{0L}(k) \cong G_0(k). \quad (11.6)$$

Consequently, if the mapping

$$L_{\{a|\mathbf{t}\}} \rightarrow D(L_{\{a|\mathbf{t}\}}) \quad (11.7)$$

provides an irreducible matrix representation of the group G_L (or \mathcal{T}_L , \mathcal{K}_L , G_{0L} , $G_{0L}(k)$), then the mapping

$$\{a|\mathbf{t}\} \rightarrow D(\{a|\mathbf{t}\}) \equiv D(L_{\{a|\mathbf{t}\}^{-1}}) = D^{-1}(L_{\{a|\mathbf{t}\}}) \quad (11.8)$$

provides an irreducible matrix representation of the group G (or \mathcal{T} , \mathcal{K} , G_0 , $G_0(k)$).

Hence to obtain matrix representations of G (or \mathcal{T} , etc.) from those of G_L , and vice versa, one must either relabel the matrices according to the mapping (11.5) or take inverses of the representation matrices.

If we express equation (8.6) using Slater's conventions and the mappings (11.5) and (11.8) we obtain

$$\begin{aligned} \phi_{ij}^{(\alpha)} &= \sum_{\mathcal{X}_L} D_{ij}^{(\alpha)*}(L_{\{b|\mathbf{t}\}^{-1}}) L_{\{b|\mathbf{t}\}^{-1}} \psi \\ &= \sum_{\mathcal{X}_L} D_{ij}^{(\alpha)*}(L_{\{b|\mathbf{t}\}}) L_{\{b|\mathbf{t}\}} \psi, \end{aligned}$$

so that the same basis functions $\phi_{ij}^{(\alpha)}$ serve for the representation (11.7) of G_L (or \mathcal{K}_L) and the representation (11.8) of G (or \mathcal{K}).

The tables of the ray representations of the point groups given in the appendix to this paper are quite independent of the convention adopted in equation (11·1); they may be used in conjunction with Slater's work, the factor system of the ray representation being provided by Slater's 'multiplication table for successive operations on a plane wave'. Indeed a number of the tables in the appendix have been checked against Slater's results in this way. The spin representations may also be incorporated in the Slater theory simply by introducing appropriate minus signs from tables 1 and 2. If tables 1 and 2 are used in conjunction with Slater's conventions, it must be remembered that it is the mapping (11·5) (with $\mathbf{t} = 0$) which provides an isomorphism between G_{0L} and G_0 and *not* the mapping (11·2).†

12. SUMMARY

The steps required to derive all the irreducible representations of a given space group G may be summarized as follows.

(i) If G is symmorphic equation (6·7) and the tables of McWeeny (1963) give the irreducible representations of \mathcal{H} for all \mathbf{k} vectors within or on the surface of the Brillouin zone. The additional representations of the double groups \mathcal{H}_d are also given by equation (6·7), where $\Gamma(b)$ is now an additional representation of the double point group $G_{0d}(k)$. The required additional representation of the 32 double-point groups may either be generated from the basis functions listed by Koster *et al.* (1963) or derived by the method of ray representations (cf. § 9, examples 3 and 4).

(ii) If G is non-symmorphic the irreducible representations of \mathcal{H} and \mathcal{H}_d for \mathbf{k} vectors within the Brillouin zone are still given by equation (6·7). For \mathbf{k} vectors on the surface of the Brillouin zone we proceed as follows.

(iii) Determine all \mathbf{k} vectors equivalent to the one under consideration and deduce $G_0(k)$.

(iv) From tables A 0 to A 11 obtain the generators a, b, \dots , of $G_0(k)$ and identify these with a_1, a_2, \dots of table 1 or b_1, b_2, \dots of table 2.

(v) Incorporate minimal non-primitive translations into a, b, \dots to obtain the generators $\{a\}, \{b\}, \dots$ of the reduced set $\{G_0(k)\}$. These minimal non-primitive translations may be obtained from the *International tables* (1953).

(vi) Evaluate the algebra of the generators of $\{G_0(k)\}$ by the use of equations (4·7), (4·8), (6·4), table 1 (or 2) and figure 1 (or 2).

(vii) Identify this algebra either with the usual point-group algebra or with an algebra listed explicitly in tables A 1 to A 11 for A, B, \dots , a gauge transformation being used if necessary. This provides an identification of the generators $\{a\}, \{b\}, \dots$ of $\{G_0(k)\}$ with the labels A, B, \dots of the matrices.

(viii) Extend the identification to all elements of $\{G_0(k)\}$.

(ix) The identification for the spin representations of \mathcal{H} is the product of the identifications for \mathcal{H} without spin and for the spin representations of $G_0(k)$.

(x) If at step (vii) or (ix) the usual point-group algebra was obtained, read off the matrices from the tables of McWeeny (1963), if not use the appropriate table A 1 ... A 11. In order to obtain all the representations one must use the arbitrary factors listed for

† It appears to the author that Slater's treatment of the cubic point groups is inconsistent with his treatment of the non-cubic point groups and space groups. In particular figure A12-4 and equations A12-67 of Slater (1963) appear to follow the Wigner convention (8·1) (with $\mathbf{t} = 0$) rather than (11·1).

A, B, \dots Equation (2.5) provides a test for the completeness of a set of irreducible representations.

(xi) The ray representations obtained at step (x) may be extended to full matrix representations of \mathcal{K} and G , or \mathcal{K}_a and G_a , using equations (7.1), (7.2) and theorems 2 and 4. However, for many purposes, including the construction of basis functions, these extensions are unnecessary; the matrices of the ray representations are sufficient (equation (8.11)).

The derivation of the matrices for all irreducible representations of all space groups and double-space groups by the method of ray representations is a much less formidable task than is suggested by a quick glance at the above (xi) step programme. Nearly all representations of nearly all space groups may be written down immediately from McWeeny's (1963) tables or appear as the result of quite trivial manipulations. There remain relatively few more complex cases; \mathbf{k} vectors of high symmetry on the surface of the Brillouin zone. Even here the required identifications are made quite easily and quickly as shown in § 9. Indeed table 4, § 9, gives explicit identifications for all the most complex cases where $G_0(k) = O_n$.

13. RELATION TO KOVALEV'S WORK

In this paper the derivation of the space group representations has been based on the fact that the matrices $D(\{b\})$ which represent the reduced set $\{G_0(k)\}$ provide a ray representation of the point group $G_0(k)$ with the factor system.

$$\lambda(b_i, b_j) = \exp(-i\mathbf{k} \cdot \mathbf{R}_n(i, j)), \quad (13.1)$$

where
$$\mathbf{R}_n(i, j) = b_i \mathbf{v}(b_j) + \mathbf{v}(b_i) - \mathbf{v}(b_i b_j). \quad (13.2)$$

If we apply the gauge transformation

$$D(\{b_i\}) \equiv D(\{b_i | \mathbf{v}(b_i)\}) = \exp(-i\mathbf{k} \cdot \mathbf{v}(b_i)) \hat{D}(b_i) \quad (13.3)$$

to the matrices $D(\{b_i\})$, the transformation of the factor system is given by the equation (cf. equation (2.6))

$$\hat{\lambda}(b_i, b_j) = \frac{\exp(-i\mathbf{k} \cdot \mathbf{v}(b_i b_j))}{\exp(-i\mathbf{k} \cdot (\mathbf{v}(b_i) + \mathbf{v}(b_j)))} \lambda(b_i, b_j). \quad (13.4)$$

We may use equations (13.1) and (13.2) to reduce $\hat{\lambda}(b_i, b_j)$ to the two equivalent forms

$$\hat{\lambda}(b_i, b_j) = \exp(-i\mathbf{k} \cdot (b_i \mathbf{v}(b_j) - \mathbf{v}(b_j))) \quad (13.5)$$

$$= \exp(-i(b_i^{-1} \mathbf{k} - \mathbf{k}) \cdot \mathbf{v}(b_j)). \quad (13.6)$$

The matrices $\hat{D}(b_i)$ of equation (13.3), or their similarity transforms, are those tabulated by Kovalev (1961). They provide a ray representation of $G_0(k)$ with the factor system (13.5), (13.6), which is projective equivalent to the ray representation $D(\{b_i\})$.

Kovalev's factor system (13.5), (13.6) is somewhat simpler than that given by (13.1) and (13.2); it involves only one non-primitive translation instead of three and gives fewer non-trivial factors. Indeed, from the alternative expressions (13.5) and (13.6) we see that

$$\hat{\lambda}(b_i, b_j) = 1$$

whenever: (i) $\mathbf{v}(b_j) = 0$, or (ii) the rotation b_i leaves $\mathbf{v}(b_j)$ invariant, or (iii) the rotation b_i^{-1} (or b_i) leaves \mathbf{k} invariant, that is does not transform \mathbf{k} into an equivalent vector of reciprocal space, or (iv) the wave vector \mathbf{k} is orthogonal to the vector $b_i \mathbf{v}(b_j) - \mathbf{v}(b_j)$.

The matrices $\hat{D}(b_i)$ have a useful property of invariance which is not shared by the

$D(\{b_i\})$. If the minimal non-primitive translation $\mathbf{v}(b_i)$ associated with b_i in the reduced set $\{G_0(k)\}$ is altered by the addition of the primitive translation \mathbf{R}_p

$$\mathbf{v}(b_i) \rightarrow \mathbf{v}(b_i) + \mathbf{R}_p$$

the associated transformation of the matrix $D(\{b_i\})$ is

$$D(\{b_i\}) \rightarrow \exp(-i\mathbf{k} \cdot \mathbf{R}_p) D(\{b_i\}),$$

whereas the matrix $\hat{D}(b_i)$ is invariant

$$\hat{D}(b_i) \rightarrow \hat{D}(b_i).$$

These properties of the factor system (13.5), (13.6) and the matrices make it practicable to tabulate the matrices $\hat{D}(b_i)$, and the corresponding matrices for the spin representations, explicitly for all space groups and all \mathbf{k} vectors. This is what Kovalev (1961) has done; his tables are still very extensive, of course, and occupy some 150 pages. The methods described in §9 enable one to obtain the same results almost as easily from the much briefer tables contained in the appendix to this paper, and tables of the vector representations of the point groups (McWeeny 1963).

In order to construct projection operators from the matrices $D(b)$ we must restore the factor removed by the gauge transformation (13.3). The expression (8.11) for the basis function $\phi_{ij}^{(\alpha)}$ is then

$$\phi_{ij}^{(\alpha)} = \sum_b \exp(i\mathbf{k} \cdot \mathbf{v}(b)) \hat{D}_{ij}^{(\alpha)*}(b) \{b | \mathbf{v}(b)\} \phi_{\mathbf{k}}. \quad (13.7)$$

As is the case with Slater's (1965) conventions, the tables A 1 to A 11 may be used to derive Kovalev's matrices $\hat{D}(a_i)$ using the factor system (13.5). The identifications are obtained somewhat more simply using this factor system, but this gain is nearly balanced by the labour of restoring the factors $\exp i\mathbf{k} \cdot \mathbf{v}(b)$ in the gauge transformation (13.3). The principal advantage of the gauge transformation (13.3) lies in the condensation of explicit tables of matrix elements.

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APPENDIX. TABLES A 0 TO A 11

Tables A 0 ... A 11 give the following information for each of the non-cyclic point groups:

(i) A set of generators a, b, \dots , and their geometric interpretation; (n) denotes an n -fold rotation axis, (\bar{n}) an n -fold rotation-reflexion axis, m a mirror plane and i the inversion.

(ii) The algebra satisfied by the generators. Apart from relations of the form $a^n = e$ (e the unit element) specifying the order of each generator, the algebraic relations given are just sufficient to permit the re-expression of any product of the generators in alphabetical order; all distinct products of the generators in alphabetical order, and e itself, give the elements of the point group.

(iii) The possible non-associated algebras satisfied by the matrices A, B, \dots , of a ray representation of the point group (except for tables A 0, where all possible algebras are associated with the usual point-group algebra).

(iv) Arbitrary factors for the generators A, B, \dots (cf. (v)).

(v) The full matrices of all non-trivial, irreducible, ray representations of the point group. These matrices are labelled by products of the matrices A, B, \dots , representing the generators. Only some of the ray representations appear explicitly in the tables. All others are obtained from these by using the listed arbitrary factors for the generators. For example, if an arbitrary factor c appears for A , A may be replaced by cA in all the products of generators which label the matrices. If the character of any element is changed by this replacement we have a new representation; otherwise we have a similarity transform of the original representation. Equation (2.5) provides a check which indicates when all inequivalent, irreducible, ray representations with the appropriate factor system have been obtained.

TABLE A 0

D_3	C_{3v}
$a = (3)$ $b = (2) \perp a$	$a = (3)$ $b = m/a$
$a^3 = e$ $b^2 = e; \quad ba = a^2b$	$A^3 = E$ $B^2 = E, \quad BA = A^2B$

TABLE A 1

C_{2v}	C_{2h}	D_2		
$a = (2)$ $b = m/a$	$a = (2)$ $b = m \perp a$	$a = (2)$ $b = (2) \perp a$		
$a^2 = e$ $b^2 = e; \quad ba = ab$	$A^2 = E; \quad \alpha = \pm 1$ $B^2 = E; \quad BA = \alpha AB$			
arbitrary factors ± 1 for A and B .				
$\alpha = -1$	E	A	B	AB
$(\Gamma_1)_{11}$	1	0	1	0
$(\Gamma_1)_{21}$	0	1	0	1
$(\Gamma_1)_{12}$	0	1	0	-1
$(\Gamma_1)_{22}$	1	0	-1	0
$\chi(\Gamma_1)$	2	0	0	0

TABLE A 2

C_{4v}		D_4				D_{2d}			
$a = (4)$ $b = m//a$		$a = (4)$ $b = (2) \perp a$				$a = (\bar{4})$ $b = (2) \perp a$			
$a^4 = e$ $b^2 = e; \quad ba = a^3b$		$A^4 = \alpha E; \quad \alpha = \pm 1$ $B^2 = E; \quad BA = A^3B$							
arbitrary factors ± 1 for A and B									
$\alpha = -1$	E	A	A^2	A^3	B	AB	A^2B	A^3B	
$(\Gamma_1)_{11}$	1	u	0	u	0	u	-1	$-u$	
$(\Gamma_1)_{21}$	0	$-u$	1	u	1	u	0	u	
$(\Gamma_1)_{12}$	0	u	-1	$-u$	1	u	0	u	
$(\Gamma_1)_{22}$	1	u	0	u	0	$-u$	1	u	
$\chi(\Gamma_1)$	2	$i\sqrt{2}$	0	$i\sqrt{2}$	0	0	0	0	

$$u = i/\sqrt{2}.$$

TABLE A 3

C_{4h}									
$a = (4)$ $b = m \perp a$		$a^4 = e$ $b^2 = e; \quad ba = ab$				$A^4 = E; \quad \alpha = \pm 1$ $B^2 = E; \quad BA = \alpha AB$			
arbitrary factors $\pm 1, \pm i$ for A ; ± 1 for B									
$\alpha = -1$	E	A	A^2	A^3	B	AB	A^2B	A^3B	
$(\Gamma_1)_{11}$	1	1	1	1	0	0	0	0	
$(\Gamma_1)_{21}$	0	0	0	0	1	-1	1	-1	
$(\Gamma_1)_{12}$	0	0	0	0	1	1	1	1	
$(\Gamma_1)_{22}$	1	-1	1	-1	0	0	0	0	
$\chi(\Gamma_1)$	2	0	2	0	0	0	0	0	

TABLE A 4

D_{2h}								
$a = m$ $b = m \perp a$ $c = m \perp a, \perp b$	$a^2 = e$ $b^2 = e; \quad ba = ab$ $c^2 = e; \quad ca = ac; \quad cb = bc$				$A^2 = E$ $B^2 = E; \quad BA = \gamma AB$ $C^2 = E; \quad CA = \beta AC; \quad CB = \alpha BC$	$\alpha = \pm 1$ $\beta = \pm 1$ $\gamma = \pm 1$		
arbitrary factors ± 1 for $A, B,$ and C								
$\alpha = -1, \beta = 1, \gamma = 1$	E	A	B	C	AB	BC	CA	ABC
$(\Gamma_1)_{11}$	1	1	1	0	1	0	0	0
$(\Gamma_1)_{21}$	0	0	0	1	0	-1	1	-1
$(\Gamma_1)_{12}$	0	0	0	1	0	1	1	1
$(\Gamma_1)_{22}$	1	1	-1	0	-1	0	0	0
$\chi(\Gamma_1)$	2	2	0	0	0	0	0	0
$\alpha = 1, \beta = -1, \gamma = 1$								
$(\Gamma_1)_{11}$	1	1	1	0	1	0	0	0
$(\Gamma_1)_{21}$	0	0	0	1	0	1	1	-1
$(\Gamma_1)_{12}$	0	0	0	1	0	1	-1	1
$(\Gamma_1)_{22}$	1	-1	1	0	-1	0	0	0
$\chi(\Gamma_1)$	2	0	2	0	0	0	0	0
$\alpha = 1, \beta = 1, \gamma = -1$								
$(\Gamma_1)_{11}$	1	1	0	1	0	0	1	0
$(\Gamma_1)_{21}$	0	0	1	0	-1	1	0	-1
$(\Gamma_1)_{12}$	0	0	1	0	1	1	0	1
$(\Gamma_1)_{22}$	1	-1	0	1	0	0	-1	0
$\chi(\Gamma_1)$	2	0	0	2	0	0	0	0
$\alpha = 1, \beta = -1, \gamma = -1$								
$(\Gamma_1)_{11}$	1	0	1	1	0	1	0	0
$(\Gamma_1)_{21}$	0	1	0	0	1	0	-1	1
$(\Gamma_1)_{12}$	0	1	0	0	-1	0	1	1
$(\Gamma_1)_{22}$	1	0	-1	-1	0	1	0	0
$\chi(\Gamma_1)$	2	0	0	0	0	2	0	0
$\alpha = -1, \beta = 1, \gamma = -1$								
$(\Gamma_1)_{11}$	1	1	0	1	0	0	1	0
$(\Gamma_1)_{21}$	0	0	1	0	-1	1	0	-1
$(\Gamma_1)_{12}$	0	0	1	0	1	-1	0	-1
$(\Gamma_1)_{22}$	1	-1	0	-1	0	0	1	0
$\chi(\Gamma_1)$	2	0	0	0	0	0	2	0
$\alpha = -1, \beta = -1, \gamma = 1$								
$(\Gamma_1)_{11}$	1	1	1	0	1	0	0	0
$(\Gamma_1)_{21}$	0	0	0	1	0	-1	1	1
$(\Gamma_1)_{12}$	0	0	0	1	0	1	-1	1
$(\Gamma_1)_{22}$	1	-1	-1	0	1	0	0	0
$\chi(\Gamma_1)$	2	0	0	0	2	0	0	0
$\alpha = -1, \beta = -1, \gamma = -1$								
$(\Gamma_1)_{11}$	1	1	0	0	0	1	0	1
$(\Gamma_1)_{21}$	0	0	1	1	-1	0	1	0
$(\Gamma_1)_{12}$	0	0	1	-1	1	0	1	0
$(\Gamma_1)_{22}$	1	-1	0	0	0	-1	0	1
$\chi(\Gamma_1)$	2	0	0	0	0	0	0	2

TABLE A 5

C_{6v}	D_6	D_{3d}	D_{3h}									
$a = (6)$ $b = m//a$	$a = (6)$ $b = (2) \perp a$	$a = (\bar{6})$ $b = m//a$	$a = (\bar{3})$ $b = m//a$									
$a^6 = e$ $b^2 = e; \quad ba = a^5b$		$A^6 = E$ $B^2 = E; \quad BA = \alpha A^5B$										
arbitrary factors ± 1 for A and B												
$\alpha = -1$	E	A	A^2	A^3	A^4	A^5	B	AB	A^2B	A^3B	A^4B	A^5B
$(\Gamma_1)_{11}$	1	1	1	1	1	1	0	0	0	0	0	0
$(\Gamma_1)_{21}$	0	0	0	0	0	0	1	-1	1	-1	1	-1
$(\Gamma_1)_{12}$	0	0	0	0	0	0	1	1	1	1	1	1
$(\Gamma_1)_{22}$	1	-1	1	-1	1	-1	0	0	0	0	0	0
$\chi(\Gamma_1)$	2	0	2	0	2	0	0	0	0	0	0	0
$(\Gamma_2)_{11}$	1	ω	ω^2	1	ω	ω^2	0	0	0	0	0	0
$(\Gamma_2)_{21}$	0	0	0	0	0	0	1	$-\omega^2$	ω	-1	ω^2	$-\omega$
$(\Gamma_2)_{12}$	0	0	0	0	0	0	1	ω	ω^2	1	ω	ω^2
$(\Gamma_2)_{22}$	1	$-\omega^2$	ω	-1	ω^2	$-\omega$	0	0	0	0	0	0
$\chi(\Gamma_2)$	2	$i\sqrt{3}$	-1	0	-1	$-i\sqrt{3}$	0	0	0	0	0	0

$\omega = e^{\frac{2}{3}\pi i}$

TABLE A 6

C_{6h}	$a = (6)$ $b = m \perp a$	$a^6 = e$ $b^2 = e; \quad ba = ab$	$A^6 = E; \quad \alpha = \pm 1$ $B^2 = E; \quad BA = \alpha AB$									
Arbitrary factors 1, $\eta = e^{\frac{1}{3}\pi i}, \eta^2, \eta^3, \eta^4, \eta^5$ for A ; ± 1 for B .												
$\alpha = -1$	E	A	A^2	A^3	A^4	A^5	B	AB	A^2B	A^3B	A^4B	A^5B
$(\Gamma_1)_{11}$	1	1	1	1	1	1	0	0	0	0	0	0
$(\Gamma_1)_{21}$	0	0	0	0	0	0	1	-1	1	-1	1	-1
$(\Gamma_1)_{12}$	0	0	0	0	0	0	1	1	1	1	1	1
$(\Gamma_1)_{22}$	1	-1	1	-1	1	-1	0	0	0	0	0	0
$\chi(\Gamma_1)$	2	0	2	0	2	0	0	0	0	0	0	0

TABLE A 7

T and T_h	$a = (2)$ $b = (2) \perp a$ $c = (3)$ at 55° to a and b $i =$ inversion (only for T_h)	$a^2 = e$ $b^2 = e; \quad ba = ab$ $c^3 = e; \quad ca = bc; \quad cb = abc$ $i^2 = e; \quad ia = ai; \quad ib = bi; \quad ic = ci$	$A^2 = \alpha E; \quad \alpha = \pm 1$ $B^2 = \alpha E; \quad BA = \alpha AB$ $C^3 = E; \quad CA = BC; \quad CB = ABC$ $I^2 = E; \quad IA = AI; \quad IB = BI; \quad IC = CI$									
arbitrary factors 1, $\omega = e^{\frac{2}{3}\pi i}, \omega^2$ for C ; ± 1 for I												
$\alpha = -1$ (for T_h only)	E EI	A AI	B BI	AB ABI	C CI	AC ACI	BC BCI	ABC $ABCI$	C^2 C^2I	AC^2 AC^2I	BC^2 BC^2I	ABC^2 ABC^2I
$(\Gamma_1)_{11}$	1	a	a	a	ω^2	$a\omega^2$	$a\omega^2$	$a\omega^2$	ω	$a\omega$	$a\omega$	$a\omega$
$(\Gamma_1)_{21}$	0	b	$b\omega^2$	$b\omega$	0	$b\omega^2$	$b\omega$	b	0	$b\omega$	b	$b\omega^2$
$(\Gamma_1)_{12}$	0	b	$b\omega$	$b\omega^2$	0	$b\omega$	$b\omega^2$	b	0	$b\omega^2$	b	$b\omega$
$(\Gamma_1)_{22}$	1	$-a$	$-a$	$-a$	ω	$-a\omega$	$-a\omega$	$-a\omega$	ω^2	$-a\omega^2$	$-a\omega^2$	$-a\omega^2$
$\chi(\Gamma_1)$	2	0	0	0	-1	1	1	1	-1	-1	-1	-1

$\omega = e^{\frac{2}{3}\pi i}, \quad a = i/\sqrt{3}, \quad b = i\sqrt{\frac{2}{3}}$

TABLE A 8

D_{4h}																
$a = (4)$	$a^4 = e$	$b = m/a$	$b^2 = e; \quad ba = a^3b$	$A^4 = \alpha E$	$B^2 = E; \quad BA = A^3B$	$C^2 = E; \quad CA = \beta AC; \quad CB = \gamma BC$	$\alpha = \pm 1$	$\beta = \pm 1$	$\gamma = \pm 1$							
$c = m \perp a$	$c^2 = e; \quad ca = ac; \quad cb = bc$	arbitrary factors ± 1 for $A, B,$ and C														
$\alpha = 1, \beta = -1, \gamma = 1$	E	A	A^2	A^3	B	AB	A^2B	A^3B	C	AC	A^2C	A^3C	BC	ABC	A^2BC	A^3BC
$(\Gamma_1)_{11}$	1	1	1	1	1	1	1	1	0	0	0	0	0	0	0	0
$(\Gamma_1)_{21}$	0	0	0	0	0	0	0	0	1	-1	1	-1	1	-1	1	-1
$(\Gamma_1)_{12}$	0	0	0	0	0	0	0	0	1	1	1	1	1	1	1	1
$(\Gamma_1)_{22}$	1	-1	1	-1	1	-1	1	-1	0	0	0	0	0	0	0	0
$\chi(\Gamma_1)$	2	0	2	0	2	0	2	0	0	0	0	0	0	0	0	0
$(\Gamma_2)_{11}$	1	0	-1	0	-1	0	1	0	-1	0	1	0	1	0	-1	0
$(\Gamma_2)_{21}$	0	i	0	-i	0	-i	0	i	0	-i	0	i	0	i	0	-i
$(\Gamma_2)_{12}$	0	i	0	-i	0	i	0	-i	0	i	0	-i	0	i	0	-i
$(\Gamma_2)_{22}$	1	0	-1	0	1	0	-1	0	1	0	-1	0	1	0	-1	0
$\chi(\Gamma_2)$	2	0	-2	0	0	0	0	0	0	0	0	0	2	0	-2	0
$\alpha = 1, \beta = 1, \gamma = -1$																
$(\Gamma_1)_{11}$	1	1	1	1	1	1	1	1	0	0	0	0	0	0	0	0
$(\Gamma_1)_{21}$	0	0	0	0	0	0	0	0	1	1	1	1	-1	-1	-1	-1
$(\Gamma_1)_{12}$	0	0	0	0	0	0	0	0	1	1	1	1	1	1	1	1
$(\Gamma_1)_{22}$	1	1	1	1	-1	-1	-1	-1	0	0	0	0	0	0	0	0
$\chi(\Gamma_1)$	2	2	2	2	0	0	0	0	0	0	0	0	0	0	0	0
$(\Gamma_2)_{11}$	1	0	-1	0	1	0	-1	0	0	i	0	-i	0	-i	0	i
$(\Gamma_2)_{21}$	0	i	0	-i	0	i	0	-i	1	0	-1	0	-1	0	1	0
$(\Gamma_2)_{12}$	0	i	0	-i	0	-i	0	i	1	0	-1	0	1	0	-1	0
$(\Gamma_2)_{22}$	1	0	-1	0	-1	0	1	0	0	i	0	-i	0	i	0	-i
$\chi(\Gamma_2)$	2	0	-2	0	0	0	0	0	0	2i	0	-2i	0	0	0	0
$\alpha = 1, \beta = -1, \gamma = -1$																
$(\Gamma_1)_{11}$	1	0	1	0	0	1	0	1	1	0	1	0	0	1	0	1
$(\Gamma_1)_{21}$	0	1	0	1	1	0	1	0	0	1	0	1	1	0	1	0
$(\Gamma_1)_{12}$	0	1	0	1	1	0	1	0	0	-1	0	-1	-1	0	-1	0
$(\Gamma_1)_{22}$	1	0	1	0	0	1	0	1	-1	0	-1	0	0	-1	0	-1
$\chi(\Gamma_1)$	2	0	2	0	0	2	0	2	0	0	0	0	0	0	0	0
$(\Gamma_2)_{11}$	1	0	-1	0	1	0	-1	0	0	-1	0	1	0	1	0	-1
$(\Gamma_2)_{21}$	0	1	0	-1	0	1	0	-1	1	0	-1	0	-1	0	1	0
$(\Gamma_2)_{12}$	0	-1	0	1	0	1	0	-1	1	0	-1	0	1	0	-1	0
$(\Gamma_2)_{22}$	1	0	-1	0	-1	0	1	0	0	1	0	-1	0	1	0	-1
$\chi(\Gamma_2)$	2	0	-2	0	0	0	0	0	0	0	0	0	0	2	0	-2
$\alpha = -1, \beta = 1, \gamma = 1$																
$(\Gamma_1)_{11}$	1	u	0	u	0	u	-1	$-u$	1	u	0	u	0	u	-1	$-u$
$(\Gamma_1)_{21}$	0	$-u$	1	u	1	u	0	u	0	$-u$	1	u	1	u	0	u
$(\Gamma_1)_{12}$	0	u	-1	$-u$	1	u	0	u	0	u	-1	$-u$	1	u	0	u
$(\Gamma_1)_{22}$	1	u	0	u	0	$-u$	1	u	1	u	0	u	0	$-u$	1	u
$\chi(\Gamma_1)$	2	$i\sqrt{2}$	0	$i\sqrt{2}$	0	0	0	0	2	$i\sqrt{2}$	$i\sqrt{2}$	0	0	0	0	0

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TABLE A 8(cont.)

$\alpha = -1, \beta = 1, \gamma = -1$	E	A	A^2	A^3	B	AB	A^2B	A^3B	C	AC	A^2C	A^3C	BC	ABC	A^2BC	A^3BC
$(\Gamma_1)_{11}$	1	u	0	u	0	u	-1	$-u$	0	t	i	$-t$	$-i$	t	0	t
$(\Gamma_1)_{21}$	0	$-u$	1	u	1	u	0	u	$-i$	t	0	t	0	$-t$	$-i$	t
$(\Gamma_1)_{12}$	0	u	-1	$-u$	1	u	0	u	i	$-t$	0	$-t$	0	$-t$	$-i$	t
$(\Gamma_1)_{22}$	1	u	0	u	0	$-u$	1	u	0	t	i	$-t$	i	$-t$	0	$-t$
$\chi(\Gamma_1)$	2	$i\sqrt{2}$	0	$i\sqrt{2}$	0	0	0	0	0	$\sqrt{2}$	$2i$	$-\sqrt{2}$	0	0	0	0
$\alpha = -1, \beta = -1, \gamma = 1$																
$(\Gamma_1)_{11}$	1	0	0	0	1	0	0	0	1	0	0	0	1	0	0	0
$(\Gamma_1)_{21}$	0	1	0	0	0	1	0	0	0	1	0	0	0	1	0	0
$(\Gamma_1)_{31}$	0	0	1	0	0	0	1	0	0	0	1	0	0	0	1	0
$(\Gamma_1)_{41}$	0	0	0	1	0	0	0	1	0	0	0	1	0	0	0	1
$(\Gamma_1)_{12}$	0	0	0	-1	0	-1	0	0	0	0	0	1	0	1	0	0
$(\Gamma_1)_{22}$	1	0	0	0	0	0	-1	0	-1	0	0	0	0	0	1	0
$(\Gamma_1)_{32}$	0	1	0	0	0	0	0	-1	0	-1	0	0	0	0	0	1
$(\Gamma_1)_{42}$	0	0	1	0	1	0	0	0	0	0	-1	0	-1	0	0	0
$(\Gamma_1)_{13}$	0	0	-1	0	0	0	1	0	0	0	-1	0	0	0	1	0
$(\Gamma_1)_{23}$	0	0	0	-1	0	0	0	1	0	0	0	-1	0	0	0	1
$(\Gamma_1)_{33}$	1	0	0	0	-1	0	0	0	1	0	0	0	-1	0	0	0
$(\Gamma_1)_{43}$	0	1	0	0	0	-1	0	0	0	1	0	0	0	-1	0	0
$(\Gamma_1)_{14}$	0	-1	0	0	0	0	0	-1	0	1	0	0	0	0	0	1
$(\Gamma_1)_{24}$	0	0	-1	0	1	0	0	0	0	0	1	0	-1	0	0	0
$(\Gamma_1)_{34}$	0	0	0	-1	0	1	0	0	0	0	0	1	0	-1	0	0
$(\Gamma_1)_{44}$	1	0	0	0	0	0	1	0	-1	0	0	0	0	0	-1	0
$\chi(\Gamma_1)$	4	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
$\alpha = -1, \beta = -1, \gamma = -1$																
$(\Gamma_1)_{11}$	1	$-r^3$	$-r^2$	$-r$	0	0	0	0	0	0	0	0	0	0	0	0
$(\Gamma_1)_{21}$	0	0	0	0	1	$-r$	r^2	$-r^3$	0	0	0	0	0	0	0	0
$(\Gamma_1)_{31}$	0	0	0	0	0	0	0	0	1	r^3	$-r^2$	r	0	0	0	0
$(\Gamma_1)_{41}$	0	0	0	0	0	0	0	0	0	0	0	0	-1	$-r$	$-r^2$	$-r^3$
$(\Gamma_1)_{12}$	0	0	0	0	1	$-r^3$	$-r^2$	$-r$	0	0	0	0	0	0	0	0
$(\Gamma_1)_{22}$	1	$-r$	r^2	$-r^3$	0	0	0	0	0	0	0	0	0	0	0	0
$(\Gamma_1)_{32}$	0	0	0	0	0	0	0	0	0	0	0	0	-1	$-r^3$	r^2	$-r$
$(\Gamma_1)_{42}$	0	0	0	0	0	0	0	0	1	r	r^2	r^3	0	0	0	0
$(\Gamma_1)_{13}$	0	0	0	0	0	0	0	0	1	$-r^3$	$-r^2$	$-r$	0	0	0	0
$(\Gamma_1)_{23}$	0	0	0	0	0	0	0	0	0	0	0	0	1	$-r$	r^2	$-r^3$
$(\Gamma_1)_{33}$	1	r^3	$-r^2$	r	0	0	0	0	0	0	0	0	0	0	0	0
$(\Gamma_1)_{43}$	0	0	0	0	-1	$-r$	$-r^2$	$-r^3$	0	0	0	0	0	0	0	0
$(\Gamma_1)_{14}$	0	0	0	0	0	0	0	0	0	0	0	0	1	$-r^3$	$-r^2$	$-r$
$(\Gamma_1)_{24}$	0	0	0	0	0	0	0	0	1	$-r$	r^2	$-r^3$	0	0	0	0
$(\Gamma_1)_{34}$	0	0	0	0	-1	$-r^3$	r^2	$-r$	0	0	0	0	0	0	0	0
$(\Gamma_1)_{44}$	1	r	r^2	r^3	0	0	0	0	0	0	0	0	0	0	0	0
$\chi(\Gamma_1)$	4	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0

$$t = \frac{1}{\sqrt{2}}, \quad u = \frac{1}{\sqrt{2}}i, \quad r = e^{i\pi} = \frac{1}{\sqrt{2}}(1+i)$$

TABLE A 9

T_d		0																								
$a = (2) \perp a$ $b = (2) \perp a$ $c = (3)$ at 55° to a and b $d = (2) \parallel$ external bisector of a and b		$A^2 = \alpha E$ $B^2 = \alpha E$; $BA = \alpha AB$ $C^3 = E$; $CA = BC$; $CB = ABC$ $D^2 = E$; $DA = \alpha BD$; $DB = \alpha AD$; $DC = C^2 D$ $\alpha = \pm 1$																								
$a^2 = e$ $b^2 = e$; $ba = ab$ $c^3 = e$; $ca = bc$; $cb = abc$ $d^2 = e$; $da = bd$; $db = ad$; $dc = c^2 d$		arbitrary factors ± 1 for D																								
α	T_d	E	A	B	AB	C	C^2	AC	BC	ABC	AC^2	BC^2	ABC^2	D	CD	$C^2 D$	AD	$ABCD$	$BC^2 D$	BD	ACD	$ABC^2 D$	ABD	BCD	$AC^2 D$	
$\alpha = -1$	$(\Gamma_1)_{11}$	1	i	0	0	-p	-q	q	q	p	-p	-q	-p	t	-t	0	u	u	-s	-u	-u	-r	t	t	t	0
	$(\Gamma_1)_{21}$	0	0	i	1	-p	-q	-q	q	-p	q	-p	-q	-t	-u	r	u	-t	0	u	-t	0	t	-u	-u	s
$\alpha = +1$	$(\Gamma_1)_{12}$	0	0	i	-1	q	-q	p	-p	q	-p	q	p	-t	u	s	-u	-t	0	-u	-t	0	t	u	r	0
	$(\Gamma_1)_{22}$	1	-i	0	0	-q	-p	p	p	q	-q	-p	-q	-t	-u	r	u	u	r	-u	-u	s	-t	-t	-t	0
$\chi(\Gamma_1)$	$\chi(\Gamma_1)$	2	0	0	-1	-1	-1	1	1	1	-1	-1	-1	0	0	0	i\sqrt{2}	i\sqrt{2}	i\sqrt{2}	-i\sqrt{2}	-i\sqrt{2}	-i\sqrt{2}	0	0	0	0
	$(\Gamma_2)_{11}$	1	0	0	0	1	1	0	0	0	0	0	0	-1	-1	-1	0	0	0	0	0	0	0	0	0	0
$\alpha = +1$	$(\Gamma_2)_{21}$	0	i	0	0	0	0	i	0	0	i	0	0	0	0	0	-i	0	0	0	-i	0	0	0	0	0
	$(\Gamma_2)_{31}$	0	0	i	0	0	0	0	i	0	0	0	i	0	0	0	0	0	0	-i	0	0	0	0	0	0
$\alpha = +1$	$(\Gamma_2)_{41}$	0	0	0	i	0	0	0	0	i	0	0	0	i	0	0	0	-i	0	0	0	-i	0	0	0	0
	$(\Gamma_2)_{12}$	0	i	0	0	0	0	0	i	0	0	0	0	0	0	0	0	0	i	0	0	0	0	0	0	i
$\alpha = +1$	$(\Gamma_2)_{22}$	1	0	0	0	1	1	0	0	-1	0	1	0	0	0	1	0	0	0	0	0	0	0	-1	1	0
	$(\Gamma_2)_{32}$	0	0	0	1	1	0	0	0	0	-1	0	0	0	0	0	0	0	0	0	-1	1	0	0	0	0
$\alpha = +1$	$(\Gamma_2)_{42}$	0	0	-1	0	0	1	1	0	0	0	0	0	0	1	0	1	0	0	0	0	0	0	0	0	0
	$(\Gamma_2)_{13}$	0	0	i	0	0	0	0	0	i	0	0	0	0	0	0	i	0	0	0	0	0	0	0	0	0
$\alpha = +1$	$(\Gamma_2)_{23}$	0	0	0	-1	0	1	0	1	0	0	0	0	0	0	0	0	-1	1	0	0	0	0	0	0	0
	$(\Gamma_2)_{33}$	1	0	0	0	0	0	-1	0	0	0	0	1	0	0	1	0	0	0	0	0	0	0	0	0	0
$\alpha = +1$	$(\Gamma_2)_{43}$	0	1	0	0	1	0	0	0	0	0	0	-1	0	0	1	0	0	0	0	0	0	0	0	0	0
	$(\Gamma_2)_{14}$	0	0	0	i	0	0	i	0	0	0	0	0	0	0	0	i	0	0	0	0	0	0	0	0	0
$\alpha = +1$	$(\Gamma_2)_{24}$	0	0	1	0	1	0	0	0	0	0	0	0	0	0	0	0	0	0	1	0	0	0	0	0	0
	$(\Gamma_2)_{34}$	0	-1	0	0	1	0	0	1	0	0	0	0	0	0	0	0	-1	1	0	0	0	0	0	0	0
$\alpha = +1$	$(\Gamma_2)_{44}$	1	0	0	0	0	0	0	-1	0	1	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
	$\chi(\Gamma_2)$	4	0	0	0	1	1	-1	-1	-1	1	1	1	0	0	0	0	0	0	0	0	0	0	0	0	0

$p = \frac{1}{2}(1+i)$, $q = \frac{1}{2}(1-i)$, $r = \frac{1}{\sqrt{2}}(1+i)$, $s = \frac{1}{\sqrt{2}}(1-i)$, $t = \frac{1}{\sqrt{2}}$, $u = \frac{1}{\sqrt{2}}i$

TABLE A 10

D_{6h}	$a^6 = e$ $b^2 = e; \quad ba = a^5b$ $c^2 = e; \quad ca = ac; \quad cb = bc$	$A^6 = E$ $B^2 = E; \quad BA = \alpha A^5B$ $C^2 = E; \quad CB = \beta BC; \quad CA = \gamma AC$	$\alpha = \pm 1$ $\beta = \pm 1$ $\gamma = \pm 1$
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arbitrary factors ± 1 for $A, B,$ or C

$= -1, \beta = 1, \gamma = 1$	E	A	A^2	A^3	A^4	A^5	B	AB	A^2B	A^3B	A^4B	A^5B	C	AC	A^2C
$(\Gamma_1)_{11}$	1	1	1	1	1	1	0	0	0	0	0	0	1	1	1
$(\Gamma_1)_{21}$	0	0	0	0	0	0	1	-1	1	-1	1	-1	0	0	0
$(\Gamma_1)_{12}$	0	0	0	0	0	0	1	1	1	1	1	1	0	0	0
$(\Gamma_1)_{22}$	1	-1	1	-1	1	-1	0	0	0	0	0	0	1	-1	1
$\chi(\Gamma_1)$	2	0	2	0	2	0	0	0	0	0	0	0	2	0	2
$(\Gamma_2)_{11}$	1	ω	ω^2	1	ω	ω^2	0	0	0	0	0	0	1	ω	ω^2
$(\Gamma_2)_{21}$	0	0	0	0	0	0	1	$-\omega^2$	ω	-1	ω^2	$-\omega$	0	0	0
$(\Gamma_2)_{12}$	0	0	0	0	0	0	1	ω	ω^2	1	ω	ω^2	0	0	0
$(\Gamma_2)_{22}$	1	$-\omega^2$	ω	-1	ω^2	$-\omega$	0	0	0	0	0	0	1	$-\omega^2$	ω
$\chi(\Gamma_2)$	2	$i\sqrt{3}$	-1	0	-1	$-i\sqrt{3}$	0	0	0	0	0	0	2	$i\sqrt{3}$	-1

$= 1, \beta = -1, \gamma = 1$

$(\Gamma_1)_{11}$	1	1	1	1	1	1	0	0	0	0	0	0	1	1	1
$(\Gamma_1)_{21}$	0	0	0	0	0	0	1	1	1	1	1	1	0	0	0
$(\Gamma_1)_{12}$	0	0	0	0	0	0	1	1	1	1	1	1	0	0	0
$(\Gamma_1)_{22}$	1	1	1	1	1	1	0	0	0	0	0	0	-1	-1	-1
$\chi(\Gamma_1)$	2	2	2	2	2	2	0	0	0	0	0	0	0	0	0
$(\Gamma_2)_{11}$	1	θ	θ^2	-1	$-\theta$	$-\theta^2$	0	0	0	0	0	0	1	θ	θ^2
$(\Gamma_2)_{21}$	0	0	0	0	0	0	1	$-\theta^2$	$-\theta$	-1	θ^2	θ	0	0	0
$(\Gamma_2)_{12}$	0	0	0	0	0	0	1	θ	θ^2	-1	$-\theta$	$-\theta^2$	0	0	0
$(\Gamma_2)_{22}$	1	$-\theta^2$	$-\theta$	-1	θ^2	θ	0	0	0	0	0	0	-1	θ^2	θ
$\chi(\Gamma_2)$	2	1	-1	-2	-1	1	0	0	0	0	0	0	0	$i\sqrt{3}$	$i\sqrt{3}$

$= -1, \beta = -1, \gamma = 1$

$(\Gamma_1)_{11}$	1	1	1	1	1	1	0	0	0	0	0	0	1	1	1
$(\Gamma_1)_{21}$	0	0	0	0	0	0	1	-1	1	-1	1	-1	0	0	0
$(\Gamma_1)_{12}$	0	0	0	0	0	0	1	1	1	1	1	1	0	0	0
$(\Gamma_1)_{22}$	1	-1	1	-1	1	-1	0	0	0	0	0	0	-1	1	-1
$\chi(\Gamma_1)$	2	0	2	0	2	0	0	0	0	0	0	0	0	2	0
$(\Gamma_2)_{11}$	1	ω	ω^2	1	ω	ω^2	0	0	0	0	0	0	-1	$-\omega$	$-\omega^2$
$(\Gamma_2)_{21}$	0	0	0	0	0	0	1	$-\omega^2$	ω	-1	ω^2	$-\omega$	0	0	0
$(\Gamma_2)_{12}$	0	0	0	0	0	0	1	ω	ω^2	1	ω	ω^2	0	0	0
$(\Gamma_2)_{22}$	1	$-\omega^2$	ω	-1	ω^2	$-\omega$	0	0	0	0	0	0	1	$-\omega^2$	ω
$\chi(\Gamma_2)$	2	$i\sqrt{3}$	-1	0	-1	$-i\sqrt{3}$	0	0	0	0	0	0	0	1	$i\sqrt{3}$

$= 1, \beta = 1, \gamma = -1$

$(\Gamma_1)_{11}$	1	-1	1	-1	1	-1	1	-1	1	-1	1	-1	0	0	0
$(\Gamma_1)_{21}$	0	0	0	0	0	0	0	0	0	0	0	0	1	1	1
$(\Gamma_1)_{12}$	0	0	0	0	0	0	0	0	0	0	0	0	1	-1	1
$(\Gamma_1)_{22}$	1	1	1	1	1	1	1	1	1	1	1	1	0	0	0
$\chi(\Gamma_1)$	2	0	2	0	2	0	2	0	2	0	2	0	0	0	0
$(\Gamma_2)_{11}$	1	$-\omega$	ω^2	-1	ω	$-\omega^2$	0	0	0	0	0	0	0	0	0
$(\Gamma_2)_{21}$	0	0	0	0	0	0	1	$-\omega^2$	ω	-1	ω^2	$-\omega$	0	0	0
$(\Gamma_2)_{31}$	0	0	0	0	0	0	0	0	0	0	0	0	1	ω	ω^2
$(\Gamma_2)_{41}$	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
$(\Gamma_2)_{12}$	0	0	0	0	0	0	1	$-\omega$	ω^2	-1	ω	$-\omega^2$	0	0	0
$(\Gamma_2)_{22}$	1	$-\omega^2$	ω	-1	ω^2	$-\omega$	0	0	0	0	0	0	0	0	0
$(\Gamma_2)_{32}$	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
$(\Gamma_2)_{42}$	0	0	0	0	0	0	0	0	0	0	0	0	1	ω^2	ω
$(\Gamma_2)_{13}$	0	0	0	0	0	0	0	0	0	0	0	0	1	$-\omega$	ω^2
$(\Gamma_2)_{23}$	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
$(\Gamma_2)_{33}$	1	ω	ω^2	1	ω	ω^2	0	0	0	0	0	0	0	0	0
$(\Gamma_2)_{43}$	0	0	0	0	0	0	1	ω^2	ω	1	ω^2	ω	0	0	0

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$-\epsilon$	ϵ^2	-1	ϵ	$-\omega^2$	0	0	0	0	0
0	0	0	0	0	1	$-\epsilon^2$	ϵ	-1	ϵ^2
0	0	0	0	0	0	0	0	0	$-\omega$
0	0	0	0	0	0	0	0	0	0
$-\epsilon^2$	ϵ	-1	ϵ^2	$-\epsilon$	1	$-\omega$	ω^2	-1	ω
0	0	0	0	0	0	0	0	0	$-\omega^2$
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	1	-1	1	-1	1
1	1	1	1	1	0	0	0	0	-1
-1	1	-1	1	-1	0	0	0	0	0
0	0	0	0	0	1	1	1	1	1
0	0	0	0	0	2	0	2	0	2
0	0	0	0	0	0	0	0	0	0
0	0	0	0	0	1	$-\omega^2$	ω	-1	ϵ^2
ϵ	ϵ^2	1	ϵ	ω^2	0	0	0	0	$-\omega$
0	0	0	0	0	0	0	0	0	0
0	0	0	0	0	1	$-\epsilon$	ϵ^2	-1	ω
0	0	0	0	0	0	0	0	0	$-\omega^2$
0	0	0	0	0	0	0	0	0	0
ϵ^2	ϵ	1	ϵ^2	ω	0	0	0	0	0
$-\epsilon$	ϵ^2	-1	ω	$-\omega^2$	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	0	0	0	0	1	ω^2	ω	1	ϵ^2
0	0	0	0	0	0	0	0	0	ω
$-\epsilon^2$	ϵ	-1	ϵ^2	$-\epsilon$	0	0	0	0	0
0	0	0	0	0	1	ϵ	ϵ^2	1	ω
0	0	0	0	0	0	0	0	0	ω^2
0	0	0	0	0	0	0	0	0	0

0	0	0	0	0	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
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	0	0
ϵ	ϵ^2	1	ϵ	ω^2	0	0	0	0	0
0	0	0	0	0	-1	$-\omega^2$	$-\omega$	-1	$-\omega^2$
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	-1	$-\omega$	$-\omega^2$	-1	$-\omega$
ϵ^2	ϵ	1	ϵ^2	ω	0	0	0	0	0
$-\epsilon$	ϵ^2	-1	ω	$-\omega^2$	0	0	0	0	0
0	0	0	0	0	1	$-\omega^2$	ω	-1	ϵ^2
0	0	0	0	0	0	0	0	0	$-\omega$
0	0	0	0	0	0	0	0	0	0
0	0	0	0	0	0	0	0	0	0
$-\epsilon^2$	ϵ	-1	ω^2	$-\epsilon$	1	$-\omega$	ω^2	-1	ω
0	0	0	0	0	0	0	0	0	$-\omega^2$
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	$-i$	i	$-i$	i	$-i$
$-i$	$-i$	$-i$	$-i$	$-i$	0	0	0	0	0
$-i$	i	$-i$	i	$-i$	0	0	0	0	0
0	0	0	0	0	i	i	i	i	i
0	0	0	0	0	0	$2i$	0	$2i$	0
0	0	0	0	0	0	0	0	0	0
0	0	0	0	0	$-i$	$i\omega^2$	$-i\omega$	i	$-i\omega^2$
$i\omega$	$-i\omega^2$	$-i$	$-i\omega$	$-i\omega^2$	0	0	0	0	0
0	0	0	0	0	0	0	0	0	0

$(\Gamma_2)_{11}$	1	$-\omega$	ω^2	-1	ω	$-\omega^2$	0	0	0	0	0	0	0	0	0
$(\Gamma_2)_{21}$	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
$(\Gamma_2)_{31}$	0	0	0	0	0	0	0	0	0	0	0	0	0	-i	$-i\omega$
$(\Gamma_2)_{41}$	0	0	0	0	0	0	1	ω^2	ω	1	ω^2	ω	0	0	0
$(\Gamma_2)_{12}$	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
$(\Gamma_2)_{22}$	1	$-\omega^2$	ω	-1	ω^2	$-\omega$	0	0	0	0	0	0	0	0	0
$(\Gamma_2)_{32}$	0	0	0	0	0	0	1	ω	ω^2	1	ω	ω^2	0	0	0
$(\Gamma_2)_{42}$	0	0	0	0	0	0	0	0	0	0	0	0	0	-i	$-i\omega^2$
$(\Gamma_2)_{13}$	0	0	0	0	0	0	0	0	0	0	0	0	0	i	$-i\omega$
$(\Gamma_2)_{23}$	0	0	0	0	0	0	1	$-\omega^2$	ω	-1	ω^2	$-\omega$	0	0	0
$(\Gamma_2)_{33}$	1	ω	ω^2	1	ω	ω^2	0	0	0	0	0	0	0	0	0
$(\Gamma_2)_{43}$	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
$(\Gamma_2)_{14}$	0	0	0	0	0	0	1	$-\omega$	ω^2	-1	ω	$-\omega^2$	0	0	0
$(\Gamma_2)_{24}$	0	0	0	0	0	0	0	0	0	0	0	0	i	$-i\omega^2$	$i\omega$
$(\Gamma_2)_{34}$	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
$(\Gamma_2)_{44}$	1	ω^2	ω	1	ω^2	ω	0	0	0	0	0	0	0	0	0
$\chi(\Gamma_2)$	4	0	-2	0	-2	0	0	0	0	0	0	0	0	0	0

$$\omega = e^{\frac{2\pi i}{3}}, \quad \theta = e^{\frac{4\pi i}{3}}$$

0	0	0	0	0	0	0	0	0	0	0
0	0	0	0	0	-i	iω ²	-iω	i	-iω ²	iω
iω	-iω ²	-i	-iω	-iω ²	0	0	0	0	0	0
0	0	0	0	0	0	0	0	0	0	0
0	0	0	0	0	-i	iω	-iω ²	i	-iω	iω ²
0	0	0	0	0	0	0	0	0	0	0
0	0	0	0	0	0	0	0	0	0	0
iω ²	-iω	-i	-iω ²	-iω	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
0	0	0	0	0	0	0	0	0	0	0
0	0	0	0	0	i	iω ²	iω	i	iω ²	iω
0	0	0	0	0	0	0	0	0	0	0
iω ²	iω	-i	iω ²	-iω	0	0	0	0	0	0
0	0	0	0	0	i	iω	iω ²	i	iω	iω 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	0	0	0	0	0	0	0

O_h	$a^2 = e$ $b^2 = e; \quad ba = ab$ $c^2 = e; \quad ca = bc; \quad cb = abc$ $d^2 = e; \quad da = bd; \quad db = ad; \quad dc = c^2d$ $i^2 = e; \quad ia = ai; \quad ib = bi; \quad ic = ci; \quad id = di$	$A^2 = \alpha E$ $B^2 = \alpha E; \quad BA = \alpha AB$ $C^2 = E; \quad CA = BC;$ $D^2 = E; \quad DA = \alpha BD;$ $I^2 = E; \quad IA = AI; \quad II$ Arbitrary factors ± 1 for L
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$\alpha = 1, \beta = -1$	E	A	B	AB	C	C^2	AC	BC	ABC	AC^2	BC^2	ABC^2	D	CD	C^2D	AD
$(\Gamma_1)_{11}$	1	1	1	1	1	1	1	1	1	1	1	1	0	0	0	0
$(\Gamma_1)_{21}$	0	0	0	0	0	0	0	0	0	0	0	0	i	i	i	i
$(\Gamma_1)_{12}$	0	0	0	0	0	0	0	0	0	0	0	0	-i	-i	-i	-i
$(\Gamma_1)_{22}$	1	1	1	1	1	1	1	1	1	1	1	1	0	0	0	0
$\chi(\Gamma_1)$	2	2	2	2	2	2	2	2	2	2	2	2	0	0	0	0
$(\Gamma_2)_{11}$	1	1	1	1	ω^2	ω	ω^2	ω^2	ω^2	ω	ω	ω	0	0	0	0
$(\Gamma_2)_{21}$	0	0	0	0	0	0	0	0	0	0	0	0	-1	$-\omega$	$-\omega^2$	-1
$(\Gamma_2)_{12}$	0	0	0	0	0	0	0	0	0	0	0	0	-1	$-\omega^2$	$-\omega$	-1
$(\Gamma_2)_{22}$	1	1	1	1	ω	ω^2	ω	ω	ω	ω^2	ω^2	ω^2	0	0	0	0
$\chi(\Gamma_2)$	2	2	2	2	-1	-1	-1	-1	-1	-1	-1	-1	0	0	0	0
$(\Gamma_3)_{11}$	M_1	M_2	M_3	M_4	M_5	M_9	M_7	M_8	M_6	M_{12}	M_{10}	M_{11}	0	0	0	0
$(\Gamma_3)_{21}$	0	0	0	0	0	0	0	0	0	0	0	0	$-M_1$	$-M_9$	$-M_5$	$-M_3$
$(\Gamma_3)_{12}$	0	0	0	0	0	0	0	0	0	0	0	0	$-M_1$	$-M_5$	$-M_9$	$-M_3$
$(\Gamma_3)_{22}$	M_1	M_3	M_2	M_4	M_9	M_5	M_{10}	M_{12}	M_{11}	M_8	M_7	M_6	0	0	0	0
$\chi(\Gamma_3)$	6	-2	-2	-2	0	0	0	0	0	0	0	0	0	0	0	0

$\alpha = -1, \beta = 1$	E	A	B	AB	C	C^2	AC	BC	ABC	AC^2	BC^2	ABC^2	D	CD	C^2D	AD
$(\Gamma_1)_{11}$	1	i	0	0	-p	-q	q	q	-p	-p	-q	-p	t	-t	0	u
$(\Gamma_1)_{21}$	0	0	i	1	-p	p	-q	q	-p	q	-p	-q	-t	-u	r	u
$(\Gamma_1)_{12}$	0	0	i	-1	-q	-q	p	-p	q	-p	q	p	-t	u	s	-u
$(\Gamma_1)_{22}$	1	-i	0	0	-q	-p	p	p	q	-q	-p	-q	-t	t	0	u
$\chi(\Gamma_1)$	2	0	0	0	-1	-1	1	1	1	-1	-1	-1	0	0	0	$i\sqrt{2}$
$(\Gamma_2)_{11}$	1	0	0	0	1	1	0	0	0	0	0	0	-1	-1	-1	0
$(\Gamma_2)_{21}$	0	i	0	0	0	0	i	0	0	i	0	0	0	0	0	-i
$(\Gamma_2)_{31}$	0	0	i	0	0	0	0	0	0	0	0	0	0	0	0	0
$(\Gamma_2)_{41}$	0	0	0	i	0	0	0	i	0	0	0	i	0	0	0	0
$(\Gamma_2)_{12}$	0	i	0	0	0	0	0	i	0	0	0	0	0	0	0	0
$(\Gamma_2)_{22}$	1	0	0	0	0	0	0	0	-1	0	1	0	0	0	1	0
$(\Gamma_2)_{32}$	0	0	0	1	1	0	0	0	0	-1	0	0	1	0	0	0
$(\Gamma_2)_{42}$	0	0	-1	0	0	1	1	0	0	0	0	0	0	1	0	1
$(\Gamma_2)_{13}$	0	0	i	0	0	0	0	0	i	i	0	0	0	0	0	i
$(\Gamma_2)_{23}$	0	0	0	-1	0	1	0	1	0	0	0	0	1	0	0	0
$(\Gamma_2)_{33}$	1	0	0	0	0	0	-1	0	0	0	0	0	0	1	0	0
$(\Gamma_2)_{43}$	0	1	0	0	1	0	0	0	0	0	-1	0	0	0	1	0
$(\Gamma_2)_{14}$	0	0	0	i	0	0	i	0	0	0	0	i	0	0	0	0
$(\Gamma_2)_{24}$	0	0	1	0	1	0	0	0	0	0	0	-1	0	1	0	0
$(\Gamma_2)_{34}$	0	-1	0	0	0	1	0	0	1	0	0	0	0	0	1	-1
$(\Gamma_2)_{44}$	1	0	0	0	0	0	0	-1	0	1	0	0	1	0	0	0
$\chi(\Gamma_2)$	4	0	0	0	1	1	-1	-1	-1	1	1	1	0	0	0	0

$\alpha = -1, \beta = -1$	E	A	B	AB	C	C^2	AC	BC	ABC	AC^2	BC^2	ABC^2	D	CD	C^2D	AD
$(\Gamma_1)_{11}$	1	0	0	0	1	1	0	0	0	0	0	0	-1	-1	-1	0
$(\Gamma_1)_{21}$	0	i	0	0	0	0	0	i	0	0	i	0	0	0	0	-i
$(\Gamma_1)_{31}$	0	0	i	0	0	0	0	0	0	0	0	i	0	0	0	0
$(\Gamma_1)_{41}$	0	0	0	i	0	0	0	0	i	0	0	0	0	0	0	0
$(\Gamma_1)_{12}$	0	i	0	0	0	0	0	i	0	0	0	0	0	0	0	0
$(\Gamma_1)_{22}$	1	0	0	0	0	0	0	0	-1	0	1	0	0	0	1	0
$(\Gamma_1)_{32}$	0	0	0	1	1	0	0	0	0	-1	0	0	1	0	0	0
$(\Gamma_1)_{42}$	0	0	-1	0	0	1	1	0	0	0	0	0	0	1	0	1
$(\Gamma_1)_{13}$	0	0	i	0	0	0	0	0	i	i	0	0	0	0	0	i
$(\Gamma_1)_{23}$	0	0	0	-1	0	1	0	1	0	0	0	0	1	0	0	0
$(\Gamma_1)_{33}$	1	0	0	0	0	0	-1	0	0	0	0	0	0	1	0	0
$(\Gamma_1)_{43}$	0	1	0	0	1	0	0	0	0	0	-1	0	0	0	1	0

TABLE A 11

MATHEMATICAL, PHYSICAL & ENGINEERING SCIENCES
 THE ROYAL SOCIETY OF TRANSACTIONS
 MATHEMATICAL, PHYSICAL & ENGINEERING SCIENCES
 THE ROYAL SOCIETY OF TRANSACTIONS

$\alpha = \pm 1$
 $\beta = \pm 1$
 $CB = ABC$
 $DB = \alpha AD; DC = C^2 D$
 $IB = BI; IC = CI; ID = \beta DI$
 D and I

ABCD	BC ² D	BD	ACD	ABC ² D	ABD	BCD	AC ² D	I	AI	BI	ABI	CI	C ² I	ACI	BCI	ABCI	AC ² I	BC ² I
0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
i	i	i	i	i	i	i	i	-1	-1	-1	-1	-1	-1	-1	-1	-1	-1	-1
-i	-i	-i	-i	-i	-i	-i	-i	-1	-1	-1	-1	-1	-1	-1	-1	-1	-1	-1
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	1	1	1	1	ω^2	ω	ω^2	ω^2	ω^2	ω	ω
$-\omega$	$-\omega^2$	-1	$-\omega$	$-\omega^2$	-1	$-\omega$	$-\omega^2$	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	0	0	0	0
$-\omega^2$	$-\omega$	-1	$-\omega^2$	$-\omega$	-1	$-\omega^2$	$-\omega$	0	0	0	0	0	0	0	0	0	0	0
0	0	0	0	0	0	0	0	-1	-1	-1	-1	$-\omega$	$-\omega^2$	$-\omega$	$-\omega$	$-\omega$	$-\omega^2$	$-\omega^2$
0	0	0	0	0	0	0	0	0	0	0	0	$-i\sqrt{3}$	$i\sqrt{3}$	$-i\sqrt{3}$	$-i\sqrt{3}$	$-i\sqrt{3}$	$i\sqrt{3}$	$i\sqrt{3}$
0	0	0	0	0	0	0	0	M_1	M_2	M_3	M_4	M_5	M_6	M_7	M_8	M_9	M_{12}	M_{10}
$-M_{11}$	$-M_7$	$-M_2$	$-M_{10}$	$-M_6$	$-M_4$	$-M_{12}$	$-M_8$	0	0	0	0	0	0	0	0	0	0	0
0	0	0	0	0	0	0	0	$-M_1$	$-M_3$	$-M_2$	$-M_4$	$-M_9$	$-M_5$	$-M_{10}$	$-M_{12}$	$-M_{11}$	$-M_8$	$-M_7$
$-M_6$	$-M_{10}$	$-M_3$	$-M_7$	$-M_{11}$	$-M_4$	$-M_8$	$-M_{12}$	0	0	0	0	0	0	0	0	0	0	0
0	0	0	0	0	0	0	0	$-M_1$	$-M_3$	$-M_2$	$-M_4$	$-M_9$	$-M_5$	$-M_{10}$	$-M_{12}$	$-M_{11}$	$-M_8$	$-M_7$
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	0	0	0	0	0	0	0	0	0	0
u	$-s$	$-u$	$-u$	$-r$	t	t	0	1	i	0	0	$-p$	$-q$	q	q	p	$-p$	$-q$
$-t$	0	u	$-t$	0	t	$-u$	s	0	0	i	1	$-p$	p	$-q$	q	$-p$	q	$-p$
$-t$	0	$-u$	$-t$	0	t	u	r	0	0	i	-1	q	$-q$	p	$-p$	q	$-p$	q
u	r	$-u$	$-u$	s	$-t$	$-t$	0	1	$-i$	0	0	$-q$	$-p$	p	p	q	$-q$	$-p$
$i\sqrt{2}$	$i\sqrt{2}$	$-i\sqrt{2}$	$-i\sqrt{2}$	$-i\sqrt{2}$	0	0	0	2	0	0	0	-1	-1	1	1	1	-1	-1
0	0	0	0	0	0	0	0	1	0	0	0	1	1	0	0	0	0	0
0	0	0	-i	0	0	0	-i	0	i	0	0	0	0	i	0	0	i	0
0	-i	-i	0	0	0	-i	0	0	0	i	0	0	0	0	i	0	0	i
-i	0	0	0	-i	-i	0	0	0	0	0	i	0	0	0	0	i	0	0
i	0	i	0	0	0	0	i	0	i	0	0	0	0	0	i	0	0	0
0	0	0	0	0	-1	1	0	1	0	0	0	0	0	0	0	-1	0	1
0	0	0	-1	1	0	0	0	0	0	0	1	1	0	0	0	0	-1	0
0	-1	0	0	0	0	0	0	0	0	-1	0	0	1	1	0	0	0	0
-1	0	0	0	i	0	i	0	0	0	i	0	0	0	0	i	i	0	0
0	1	0	0	0	0	0	0	0	0	0	-1	0	1	0	1	0	0	0
0	0	0	0	0	1	0	-1	1	0	0	0	0	0	-1	0	0	0	0
0	0	-1	1	0	0	0	0	0	1	0	0	1	0	0	0	0	0	-1
0	i	0	i	0	i	0	0	0	0	0	i	0	0	i	0	0	0	i
0	0	1	0	-1	0	0	0	0	0	1	0	1	0	0	0	0	0	0
1	0	0	0	0	0	0	0	0	-1	0	0	0	1	0	0	1	0	0
0	0	0	0	0	0	-1	1	1	0	0	0	0	0	0	-1	0	1	0
0	0	0	0	0	0	0	0	4	0	0	0	1	1	-1	-1	-1	1	1
0	0	0	0	0	0	0	0	0	y	y	y	0	0	y	y	y	y	y
0	0	0	-i	0	0	0	-i	x	0	x	$-x$	x	x	x	$-x$	x	0	x
0	-i	-i	0	0	0	-i	0	x	$-x$	0	x	x	x	$-x$	0	x	$-x$	0
-i	0	0	0	-i	-i	0	0	x	x	$-x$	0	x	x	$-x$	$-x$	0	x	$-x$
i	0	i	0	0	0	0	i	x	0	$-x$	x	x	x	x	0	$-x$	$-x$	x
0	0	0	0	0	-1	1	0	0	y	$-y$	$-y$	$-y$	$-y$	$-y$	y	0	y	0
0	0	0	-1	1	0	0	0	y	y	y	0	0	$-y$	$-y$	y	$-y$	0	y
0	-1	0	0	0	0	0	0	$-y$	y	0	y	y	0	$-y$	y	$-y$	$-y$	$-y$
0	0	0	0	i	0	i	0	x	x	0	$-x$	x	$-x$	x	0	0	0	$-x$
1	1	0	0	0	0	0	0	$-y$	y	y	0	y	0	y	0	y	y	$-y$
0	0	0	0	0	1	0	-1	0	$-y$	y	$-y$	$-y$	y	0	y	y	y	y
0	0	1	1	0	0	0	0	y	0	y	y	0	$-y$	$-y$	$-y$	y	y	0

BC^2I	ABC^2I	DI	CDI	C^2DI	ADI	$ABCDI$	BC^2DI	BDI	$ACDI$	ABC^2DI	$ABDI$	$BCDI$	AC^2DI
0 -1	0 -1	i 0	i 0	i 0	i 0	i 0	i 0	i 0	i 0	i 0	i 0	i 0	i 0
-1 0	-1 0	0 -i	0 -i	0 -i	0 -i	0 -i	0 -i	0 -i	0 -i	0 -i	0 -i	0 -i	0 -i
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
ω 0	ω 0	0 -1	0 $-\omega$	0 $-\omega^2$	0 -1	0 $-\omega$	0 $-\omega^2$	0 -1	0 $-\omega$	0 $-\omega^2$	0 -1	0 $-\omega$	0 $-\omega^2$
0 $-\omega^2$	0 $-\omega^2$	1 0	ω^2 0	ω 0	1 0	ω^2 0	ω 0	1 0	ω^2 0	ω 0	1 0	ω^2 0	ω 0
$i\sqrt{3}$	$i\sqrt{3}$	0	0	0	0	0	0	0	0	0	0	0	0
M_{10} 0	M_{11} 0	0 $-M_1$	0 $-M_9$	0 $-M_5$	0 $-M_3$	0 $-M_{11}$	0 $-M_7$	0 $-M_2$	0 $-M_{10}$	0 $-M_6$	0 $-M_4$	0 $-M_{12}$	0 $-M_8$
0 $-M_7$	0 $-M_6$	M_1 0	M_5 0	M_9 0	M_3 0	M_6 0	M_{10} 0	M_3 0	M_7 0	M_{11} 0	M_4 0	M_8 0	M_{12} 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 0
$-q$ $-p$	$-p$ $-q$	t $-t$	$-t$ $-u$	0 r	u u	u $-t$	$-s$ 0	$-u$ u	$-u$ $-t$	$-r$ 0	t t	t $-u$	0 s
q $-p$	p $-q$	$-t$ $-t$	u t	s 0	$-u$ u	$-t$ u	0 r	$-u$ $-u$	$-t$ $-u$	0 s	t $-t$	u $-t$	r 0
-1 0	-1 0	0 0	0 0	0 0	$i\sqrt{2}$ 0	$i\sqrt{2}$ 0	$i\sqrt{2}$ 0	$-i\sqrt{2}$ 0	$-i\sqrt{2}$ 0	$-i\sqrt{2}$ 0	0 0	0 0	0 0
0 0 i 0	0 0 0 i	-1 0 0 0	-1 0 0 0	-1 0 0 0	0 -i 0 0	0 0 0 -i	0 0 -i 0	0 0 -i 0	0 -i 0 0	0 0 0 -i	0 0 0 -i	0 0 -i 0	0 -i 0 0
0 1 0 0	i 0 0 0	0 0 1 0	0 0 0 1	0 1 0 0	0 0 0 1	i 0 0 0	0 0 0 -1	i 0 0 0	0 0 -1 0	0 0 1 0	0 -1 0 0	0 1 0 0	i 0 0 0
0 0 0 -1	0 0 1 0	0 1 0 0	0 0 1 0	0 0 0 1	i 0 0 0	0 -1 0 0	0 1 0 0	0 0 0 -1	0 0 0 1	i 0 0 0	0 0 1 0	0 0 0 0	0 0 -1 0
i 0 0 0	0 -1 0 0	0 0 0 1	0 1 0 0	0 0 1 0	0 0 -1 0	0 0 1 0	i 0 0 0	0 1 0 0	i 0 0 0	0 -1 0 0	i 0 0 0	0 0 0 -1	0 0 0 1
1 1	1 1	0 0	0 0	0 0	0 0	0 0	0 0	0 0	0 0	0 0	0 0	0 0	0 0
y x 0 $-x$	y $-x$ x 0	0 x x x	0 x x x	0 x x x	y 0 x x	y $-x$ x 0	y x 0 $-x$	y x 0 $-x$	y x 0 x	y 0 $-x$ x	y $-x$ x 0	y x 0 $-x$	y 0 x x
x 0 y $-y$	0 y y y	$-x$ y 0 $-y$	$-x$ $-y$ 0 y	$-x$ 0 $-y$ y	$-x$ $-y$ y $-y$	0 $-y$ $-y$ 0	x $-y$ $-y$ 0	0 $-y$ $-y$ 0	x $-y$ 0 y	$-x$ y 0 $-y$	x 0 y $-y$	$-x$ 0 $-y$ $-y$	0 $-y$ $-y$ $-y$
$-x$ $-y$ y 0	x $-y$ 0 y	$-x$ 0 $-y$ y	$-x$ y 0 $-y$	0 $-y$ $-y$ 0	x $-y$ y $-y$	x 0 $-y$ $-y$	$-x$ 0 $-y$ $-y$	x $-y$ $-y$ 0	$-x$ $-y$ $-y$ 0	0 y 0 $-y$	$-x$ $-y$ 0 $-y$	0 $-y$ $-y$ $-y$	x $-y$ 0 y

TABLE A 10

D_{ab} $a = (b)$ $b = m/a$ $c = m/a$		$q^a = e$ $q^b = e; bq = a^2e$ $q^c = e; ca = a; \delta = bc$						$F = E$ $F' = E; EA = xPB$ $C^2 = E; CB = \beta BC; CA = \gamma AC$						$\alpha = \pm 1$ $\beta = \pm 1$ $\gamma = \pm 1$																					
arbitrary factors ± 1 for A, B, C																																			
$\alpha = -1, \beta = 1, \gamma = 1$						$\alpha = 1, \beta = -1, \gamma = 1$						$\alpha = -1, \beta = -1, \gamma = 1$						$\alpha = 1, \beta = 1, \gamma = -1$						$\alpha = -1, \beta = 1, \gamma = -1$						$\alpha = 1, \beta = -1, \gamma = -1$					
$(\Gamma_{11})_{11}$		E	A	P	P'	P''	B	AB	AB'	AB''	AB'	AB''	C	AC	AC'	AC''	BC	BC'	BC''	BC'	BC''														
$(\Gamma_{11})_{11}$		1	1	1	1	1	1	1	1	1	1	1	1	1	1	1	1	1	1	1	1	1													
$(\Gamma_{11})_{12}$		0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0														
$(\Gamma_{11})_{21}$		0	0	0	0	0	1	1	1	1	1	1	0	0	0	0	1	1	1	1	1	1													
$(\Gamma_{11})_{22}$		1	-1	1	-1	1	-1	1	-1	1	-1	0	-1	1	-1	1	-1	1	-1	1	-1	0													
$\chi(\Gamma_1)$		2	0	2	0	2	0	0	0	0	0	2	0	2	0	2	0	0	0	0	0	0													
$(\Gamma_{21})_{11}$		1	ω	ω^2	1	ω	ω	ω^2	ω	ω^2	ω	0	1	ω	ω^2	1	ω	ω^2	1	ω	ω^2	0													
$(\Gamma_{21})_{12}$		0	0	0	0	0	1	ω	ω^2	1	ω	0	0	0	0	0	1	ω	ω^2	1	ω														
$(\Gamma_{21})_{21}$		1	ω^2	ω	-1	ω^2	ω	ω	ω^2	ω	ω^2	0	1	ω^2	ω	ω^2	1	ω	ω^2	1	ω														
$(\Gamma_{21})_{22}$		1	ω	ω^2	ω	ω^2	0	ω	ω^2	1	ω	0	0	0	0	0	0	ω	ω^2	0	ω														
$\chi(\Gamma_2)$		2	$i\sqrt{3}$	-1	0	-1	0	0	0	0	0	2	$i\sqrt{3}$	-1	0	-1	0	0	0	0	0	0													

PHILOSOPHICAL TRANSACTIONS OF THE ROYAL SOCIETY OF LONDON
 MATHEMATICAL, PHYSICAL & ENGINEERING SCIENCES

