REVIEWS OF MODERN PHYSICS VOLUME 37, NUMBER 1 JANUARY 1965

Lattice Harmonics II. Hexagonal Close-Packed Lattice

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A general discussion of the treatment of the asymmorphic space groups is given, with special reference to the hexagonal close-packed lattice ($P6_3/mmc$), for which the irreducible representations are given in full and the lattice harmonics listed for all l. The expansions possess the same properties as those given for the cubic groups in the preceding paper.

1. INTRODUCTION

We refer the reader to Secs. 1 and 2 of the preceding paper[1] (hereafter referred to as I) for a general introduction. We discuss in Sec. 2 below the derivation of lattice harmonics for asymmorphic groups. We also discuss the derivation of the irreducible representations of these groups. In particular, we give in Sec. 4 a prescription to obtain the group of the **k** vector, which is applied in Sec. 5 to the hexagonal close-packed lattice. The reduction of this group has already been carried out by Herring[2] (see also Antoncik and Trlifaj[3]) but we offer here a systematic treatment that can be used in general for asymmorphic groups, whereas Herring employed an *ad hoc* procedure. Our treatment is also more complete, since we give full matrix representations, which are, of course, essential for the specification of the lattice harmonics. The latter are given in Sec. 6 for all orders of l.

2. ASYMMORPHIC SPACE GROUPS AND LATTICE HARMONICS

In dealing with asymmorphic space groups, that is groups that contain screw axes or glide planes, the general theory reviewed in I, Sec. 2 becomes more involved on two counts: both the structure of the irreducible representations and the use of the projection operators (I.7) are more complex.

We shall first consider the irreducible representations. As mentioned in Part I, Sec. 2 these are obtained by reducing the group $\mathbf{G}^{\mathbf{k}}$ of the **k** vector. $\mathbf{G}^{\mathbf{k}}$ contains the translation group $\mathbf{\Gamma}$ as a subgroup, but in the symmorphic groups $\mathbf{\Gamma}$ can be separated out and it is enough to reduce $G^{\mathbf{k}}$, the cogroup of **k**, which is a point group. $G^{\mathbf{k}}$ is in fact the group of the coset representatives of the factor group $\mathbf{G}^{\mathbf{k}}/\mathbf{\Gamma}$. However, for asymmorphic groups these coset representatives, which are operations $\{\alpha \mid \mathbf{v}\}$, do not necessarily form a group, since the product of two of them may be an operation in $\mathbf{\Gamma}$.

The way out of this difficulty was found by Herring.[2] Let us define $\mathbf{\Gamma}^{\mathbf{k}}$ as the subgroup of operations $\{E \mid \mathbf{t}\}$ of $\mathbf{\Gamma}$ for which $\mathbf{k}\cdot\mathbf{t}=2\pi n$, where n is an integer: their representatives are unit matrices (see I.3). We write the group to be reduced as the factor group $\mathbf{G}^{\mathbf{k}}/\mathbf{\Gamma}^{\mathbf{k}}$ and in order to find its irreducible representations all the operations of $\mathbf{\Gamma}^{\mathbf{k}}$ can be assimilated with the identity. It was pointed out by Altmann[4] that the factor group $\mathbf{G}^{\mathbf{k}}/\mathbf{\Gamma}^{\mathbf{k}}$ can now be considered in a different way. Rather than taking $\mathbf{\Gamma}^{\mathbf{k}}$ to be the identity of this group, we can consider *each* element of $\mathbf{\Gamma}^{\mathbf{k}}$ to be the identity. In this way $\mathbf{G}^{\mathbf{k}}/\mathbf{\Gamma}^{\mathbf{k}}$ can be taken—when we want to find its irreducible representations—to be the "group" $\mathbf{C}^{\mathbf{k}}$ of the coset representatives that appear in it. We give the word group here in quotation marks since $\mathbf{C}^{\mathbf{k}}$ is only a group in what we shall call the Herring sense, that is when we use his extended definition of the identity. It should be noticed that whenever we have to deal with a factor group with $\mathbf{\Gamma}^{\mathbf{k}}$ we shall take it to be the group, in Herring's sense, of its coset representatives.

The group that we must reduce, $\mathbf{C}^{\mathbf{k}}$, is not in general a point group. In Sec. 4 we shall give a prescription for its derivation and in Sec. 5 we shall obtain it for all values of **k** in the hexagonal close-packed lattice.

As regards the use of the projection operators, their application to the hexagonal close-packed lattice will serve as an example of the general theory, which is an extension of the method given by Altmann.[4] We shall first require a particular property of the hexagonal close-packed lattice, which will be discussed in Sec. 3: it will be seen there that every point in this lattice is linked to its near neighbors either by a lattice translation $\{E \mid \mathbf{t}\}$ or by an inversion through the midpoint of a vector $\boldsymbol{\tau}$ which is not a vector of the lattice. This inversion operation can be written as $\{i \mid \boldsymbol{\tau}\}$. Therefore, in order to write the transform of the harmonics Y_l^m under the operators $\{\alpha \mid \mathbf{v}\}$, it is enough to define the two following operations:

$$\{E \mid \mathbf{t}\}\, Y_l^m \equiv {}^{\mathbf{t}}Y_l^m, \tag{1}$$

$$\{i \mid \boldsymbol{\tau}\}\, Y_l^m \equiv {}^{\boldsymbol{\tau}}\bar{Y}_l^m. \tag{2}$$

As in part I, ${}^{\mathbf{t}}Y_l^m$ is a spherical harmonic centered about the point **t**, whereas ${}^{\boldsymbol{\tau}}\bar{Y}_l^m$ is a harmonic about the point $\boldsymbol{\tau}$ and is such that the axes at $\boldsymbol{\tau}$ are inverted with respect to those at the origin. The bar above the symbol Y_l^m denotes this inversion.[5]

[1] S. L. Altmann and A. P. Cracknell, Rev. Mod. Phys. **37**, 19 (1965).
[2] C. Herring, J. Franklin Inst. **233**, 525 (1942).
[3] E. Antoncik and M. Trlifaj, Czechoslov. J. Phys. **1**, 97 (1952).
[4] S. L. Altmann, Proc. Roy. Soc. (London) **A244**, 141 (1958).
[5] The purpose of this choice of axes is to avoid a factor $(-1)^l$ which would otherwise appear on account of the transformation properties of the spherical harmonics under inversion.

In order to apply the operators $\{\alpha \mid \mathbf{v}\}$ on the spherical harmonics, as required when using the projection operators (I.7), we write

$$\{\alpha \mid \mathbf{t}\} \equiv \{E \mid \mathbf{t}\}\{\alpha \mid 0\}, \tag{3}$$

$$\{\alpha \mid \mathbf{v}\} \equiv \{i \mid \mathbf{v}\}\{\beta \mid 0\}, \tag{4}$$

where $\mathbf{t}$ and $\mathbf{v}$ are a lattice and a nonlattice vector, respectively, and $\beta = i\alpha$. Then:

$$\{\alpha \mid \mathbf{t}\} Y_l^m = \{E \mid \mathbf{t}\}\{\alpha \mid \mathbf{0}\} Y_l^m \tag{5}$$

$$= \{E \mid \mathbf{t}\} \sum_{m'} Y_l^{m'} D^l(\alpha)_{m'm} \tag{6}$$

$$= \sum_{m'} {}^{\mathbf{t}}Y_l^{m'} D^l(\alpha)_{m'm}. \tag{7}$$

We use in (6) the definition of the representations of the rotation group: the $D^l(\alpha)_{m'm}$ are the matrix elements of the corresponding representatives, but if the expressions of Altmann[4] or Altmann and Bradley[6] are used it is necessary to interchange α and α^{-1}, since we now consider α as an active operator.

In the same manner:

$$\{\alpha \mid \mathbf{v}\} Y_l^m = \{i \mid \mathbf{v}\}\{\beta \mid \mathbf{0}\} Y_l^m \tag{8}$$

$$= \{i \mid \mathbf{v}\} \sum_{m'} Y_l^{m'} D^l(\beta)_{m'm} \tag{9}$$

$$= \sum_{m'} {}^{\mathbf{v}}\bar{Y}_l^{m'} D^l(\beta)_{m'm}. \tag{10}$$

Expressions (7) and (10) are the basic ones required in order to use the projection operators: the result of their application will be symmetry-adapted expansions over the unit cell, from which, as in (I.10), the expansions over the whole lattice, that is the lattice harmonics, are obtained by the Bloch condition.

Considering again the representations of asymmorphic groups, it is important to recognize that the basic idea is that two translations are now considered identical if they have the same representative and that this introduces some important consequences. For instance, whereas, as is well-known in the general theory of space groups, translations commute only exceptionally with other operations, this is no longer the case in the new interpretation as shown by the following.

Theorem (Johnston,[7] p. 144). All translations commute (in the new sense) with the operations $\{\alpha \mid \mathbf{v}\}$ of $\mathbf{G}^{\mathbf{k}}$, the group of the $\mathbf{k}$ vector. Proof:

$$\{E \mid \mathbf{t}\}\{\alpha \mid \mathbf{v}\} = \{\alpha \mid \mathbf{v}+\mathbf{t}\}, \tag{11}$$

$$\{\alpha \mid \mathbf{v}\}\{E \mid \mathbf{t}\} = \{\alpha \mid \alpha\mathbf{t}+\mathbf{v}\}. \tag{12}$$

In the new interpretation $\alpha\mathbf{t}$ and $\mathbf{t}$ are identical. In fact: $D(\alpha\mathbf{t}) = \exp(-i\mathbf{k}\cdot\alpha\mathbf{t}) = \exp(-i\alpha^{-1}\mathbf{k}\cdot\mathbf{t})$. Since $\{\alpha \mid \mathbf{v}\} \in \mathbf{G}^{\mathbf{k}}$, the operation that corresponds to α^{-1} must also belong to $\mathbf{G}^{\mathbf{k}}$, and α^{-1} must also leave $\mathbf{k}$ invariant. Therefore $D(\alpha\mathbf{t}) = \exp(-i\mathbf{k}\cdot\mathbf{t}) = D(\mathbf{t})$.

[6] S. L. Altmann and C. J. Bradley, Phil. Trans. Roy. Soc. London **A255**, 199 (1963).
[7] D. F. Johnston, Rept. Progr. Phys. **23**, 66 (1960).

3. THE HEXAGONAL CLOSE-PACKED LATTICE

The hexagonal close-packed lattice is represented in Fig. 1, where the symmetry operations are identified in the standard notation for point groups: this has been chosen to agree with the nomenclature of Altmann and Bradley.[6] The black circles represent atoms in the plane of the drawing and the open circles those at a distance $c/2$ above and below this plane, where c is the length of the vertical translation vector. There are two atoms per unit cell: we go from one to the other by a translation $\boldsymbol{\tau}$ that does not belong to the translation lattice. As mentioned in Sec. 2, it is clear that every atom is linked to each of its twelve near neighbors either by a $\boldsymbol{\tau}$ translation or a translation $\mathbf{t}$ of the lattice.

The space group of this lattice is $\mathbf{D}_{6h}^4$ and its point group is $\mathbf{D}_{6h} = \mathbf{D}_{3h} \times \mathbf{C}_i$. The operations α of $\mathbf{D}_{3h}$ appear as space-group operations $\{\alpha \mid \mathbf{0}\}$, whereas i has to be transformed into $j \equiv \{i \mid \boldsymbol{\tau}\}$. If we write $\mathbf{J} = \{E \mid \mathbf{0}\} + \{i \mid \boldsymbol{\tau}\}$ the nontranslational part of the space group is given by the product of $\mathbf{D}_{3h}$ and $\mathbf{J}$. The space group itself is a product of this set with the translation group $\boldsymbol{\Gamma}$.

We show in Fig. 2 the first Brillouin zone of the lattice, which can be properly oriented with respect to the lattice vectors by comparison with Fig. 1(a). We identify in Fig. 2 all the points of symmetry as well as representative points on lines of symmetry. We do this for a region of volume equal to $\frac{1}{24}$ of the zone, although one should strictly consider the whole of the zone. As an example, although the groups $\mathbf{C}^{\mathbf{k}}$ for K and K^* [see Fig. 1(b)], for instance, are isomorphic, their representations are not identical. Nevertheless they are very simply related (see point K in Sec. 4), so that the description of the representations for the points in the basic domain of Fig. 2 is sufficient to deal with all the remaining cases. It is enough to remember that the representations of the group of the $\mathbf{k}$ vector spanned by the different vectors of a star are not identical. If characters of the representations and their

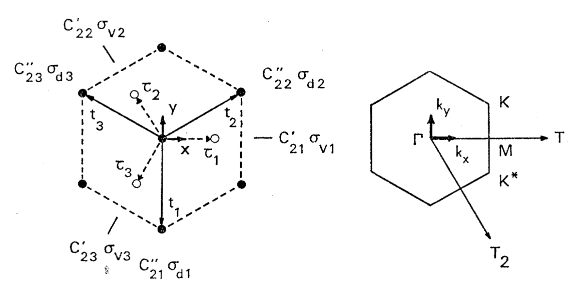

FIG. 1. The hexagonal close-packed lattice. (a) The direct lattice. $\mathbf{t}_0$ is perpendicular to the plane of the drawing. (b) The reciprocal lattice in the correct orientation and arbitrary scale. $\mathbf{T}_1$ and $\mathbf{T}_2$ are the reciprocal lattice unit vectors, $\mathbf{T}_0$ is perpendicular to the plane of the drawing. We use the definition $\mathbf{t}_i \cdot \mathbf{T}_j = 2\pi\delta_{ij}$. Γ, K, M, and K^* are important points of symmetry in $\mathbf{k}$ space.

energies only are required it is enough to deal with the basic domain of the Brillouin zone, but if the matrix representations are required, as is the case in this paper, attention must be paid to possible similarity transformations introduced for vectors outside the basic domain, as well as changes in the representatives of certain translations.

4. GENERAL METHOD FOR THE DERIVATION OF THE GROUP $\mathbf{C}^{\mathbf{k}}$

We recall that $\mathbf{C}^{\mathbf{k}}$ is the group, in Herring's sense, of coset representatives of $\mathbf{G}^{\mathbf{k}}/\mathbf{\Gamma}^{\mathbf{k}}$. We shall give a prescription to obtain this group, which will allow us at the same time to classify the various cases that appear in the hexagonal close-packed lattice. We shall use the following notation in this work: a space-group operation will be given, as before, by $\{\alpha \mid \mathbf{v}\}$, where $\mathbf{v}$ can be $\mathbf{0}$, $\boldsymbol{\tau}$ or a lattice vector $\mathbf{t}$, or any combination of these. On the other hand, $\{\alpha \mid \mathbf{w}\}$ stands for an operation in which the translational part $\mathbf{w}$ can only be $\mathbf{0}$ or $\boldsymbol{\tau}$. The latter, unless restrictions to the contrary exist, can be any of the six vectors, $\boldsymbol{\tau}_1$, $\boldsymbol{\tau}_2$, $\boldsymbol{\tau}_3$ and their reflections in the plane of Fig. 1(a).

The prescription to obtain $\mathbf{C}^{\mathbf{k}}$ is as follows:

(i) Find $\mathbf{\Gamma}^{\mathbf{k}}$.

(ii) Find $\boldsymbol{\gamma}^{\mathbf{k}} \equiv \mathbf{\Gamma}/\mathbf{\Gamma}^{\mathbf{k}}$. With our interpretation of the factor group, $\boldsymbol{\gamma}^{\mathbf{k}}$ is given by $\{E \mid \mathbf{0}\}$ plus all the different (in Herring's sense) operations of $\mathbf{\Gamma}$ not in $\mathbf{\Gamma}^{\mathbf{k}}$.

(iii) Find the subgroup $\mathbf{P}^{\mathbf{k}}$ of all the operations α_i of the point group that leave $\mathbf{k}$ invariant. Write $\mathbf{P}^{\mathbf{k}} = \sum_i \{\alpha_i \mid \mathbf{0}\}$.

(iv) Form the *set* of operations (*not* in general a group) $\mathcal{P}^{\mathbf{k}} \equiv \sum \{\alpha_i \mid \mathbf{w}_i\}$. $\{\alpha_i \mid \mathbf{w}_i\}$ is a space-group operation, but not a general one, since $\mathbf{w}_i$ cannot be a translation vector of $\mathbf{\Gamma}$ except the null one. It is useful to notice that only one $\mathbf{w}_i$ needs be associated with any one α_i. This is so because

$$\{\alpha_i \mid \mathbf{w}_j\} = \{\alpha_i \mid \mathbf{w}_i\}\{E \mid \mathbf{t}\} \tag{13}$$

for some lattice translation $\mathbf{t}$: if $\{E \mid \mathbf{t}\} \in \mathbf{\Gamma}^{\mathbf{k}}$ we take it to be the identity; if $\{E \mid \mathbf{t}\} \in \boldsymbol{\gamma}^{\mathbf{k}}$ see (v) below.

(v) Form

$$\mathbf{C}^{\mathbf{k}} = \boldsymbol{\gamma}^{\mathbf{k}} \cdot \mathcal{P}^{\mathbf{k}}, \tag{14}$$

where the dot stands for a set product. It is now clear that if, in (13), $\{E \mid \mathbf{t}\} \in \boldsymbol{\gamma}^{\mathbf{k}}$, $\{\alpha_i \mid \mathbf{w}_j\}$ appears in the product (14) and should not be listed independently in $\mathcal{P}^{\mathbf{k}}$.

(vi) Choose the $\mathbf{w}_i$'s in $\mathcal{P}^{\mathbf{k}}$ so that, *if possible*, the product of two operations of $\mathcal{P}^{\mathbf{k}}$, except possibly the identity, is never in $\boldsymbol{\gamma}^{\mathbf{k}}$. (In doing this, of course, only the operations for which $\mathbf{w}_i = \boldsymbol{\tau}$ need be considered.) The structure of $\mathbf{C}^{\mathbf{k}}$, as described in (vii), will be found during this process: when such a choice of $\mathbf{w}$'s is possible cases (A) or (B) in (vii) arise; when it is not, case (C) holds.

(vii) The structure of $\mathbf{C}^{\mathbf{k}}$ is described by the following three cases:

(A) It is possible to choose the $\mathbf{w}_i$'s so that not only the product of two operations of $\mathcal{P}^{\mathbf{k}}$ is never in $\boldsymbol{\gamma}^{\mathbf{k}}$ but also $\mathcal{P}^{\mathbf{k}}$ is a group. Then:

$$\mathbf{C}^{\mathbf{k}} = \boldsymbol{\gamma}^{\mathbf{k}} \times \mathcal{P}^{\mathbf{k}}, \tag{15}$$

where the validity of the direct product is a consequence of the theorem of Sec. 2. Since $\mathcal{P}^{\mathbf{k}}$ is isomorphic to $\mathbf{P}^{\mathbf{k}}$, which is a point group, the representations of $\mathbf{C}^{\mathbf{k}}$ follow immediately.

(B) It is possible to choose the $\mathbf{w}_i$'s so that the product of two operations of $\mathcal{P}^{\mathbf{k}}$ is never in $\boldsymbol{\gamma}^{\mathbf{k}}$ but it is inevitable that some products of operations of $\mathcal{P}^{\mathbf{k}}$ are of the form

$$\{\alpha_i \mid \mathbf{w}_i\}\{\alpha_j \mid \mathbf{w}_j\} = \{\alpha_r \mid \mathbf{w}_r + \mathbf{t}\}, \tag{16}$$

where $\{E \mid \mathbf{t}\} \in \boldsymbol{\gamma}^{\mathbf{k}}$. In this case closure can be obtained for $\mathcal{P}^{\mathbf{k}}$ by replacing some of the operations $\{\alpha \mid \mathbf{w}\}$ by $\{\alpha \mid \mathbf{w}+\mathbf{t}\}$ as required by products of the form (16). The group thereby formed will be called $\mathcal{P}_{\mathbf{t}}^{\mathbf{k}}$. Then:

$$\mathbf{C}^{\mathbf{k}} = \boldsymbol{\gamma}^{\mathbf{k}} \times \mathcal{P}_{\mathbf{t}}^{\mathbf{k}}; \tag{17}$$

$\mathcal{P}_{\mathbf{t}}^{\mathbf{k}}$ is isomorphic to $\mathbf{P}^{\mathbf{k}}$ so that the representations of $\mathbf{C}^{\mathbf{k}}$ follow immediately.

(C) For every choice of the $\mathbf{w}_i$'s there is always a pair of operations of $\mathcal{P}^{\mathbf{k}}$ such that their product belongs to $\boldsymbol{\gamma}^{\mathbf{k}}$. It is not possible in this case to express $\mathbf{C}^{\mathbf{k}}$ in a form simpler than (14).

(viii) In case (A) the class structure of $\mathbf{C}^{\mathbf{k}}$ is essentially that of $\mathbf{P}^{\mathbf{k}}$. It is important to observe that this is no longer so in cases (B) and (C): the class structure of the groups obtained must be carefully examined.

(ix) When the representations of $\mathbf{C}^{\mathbf{k}}$ are obtained, by some standard method, it should be noticed that not all of them are allowed. Only those for which the operations of $\boldsymbol{\gamma}^{\mathbf{k}}$ are correctly represented by $\exp(-i\mathbf{k}\cdot\mathbf{t})$ should be retained.

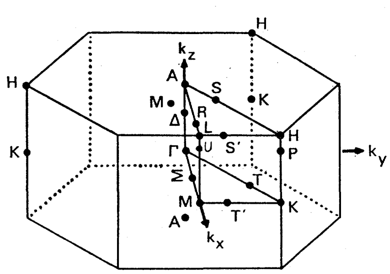

FIG. 2. The first Brillouin zone for hexagonal space groups.

5. THE GROUPS $\mathbf{C}^{\mathbf{k}}$ FOR ALL THE POINTS IN THE BRILLOUIN ZONE

We shall not go in detail through the prescription of Sec. 4 for all points in the Brillouin zone. Instead, we shall consider a sufficient number of cases so that the details of the prescription become clear. Complete details about every point can in any case be obtained with the help of the tables of characters in Sec. 6.

The coordinates of points in $\mathbf{k}$ space will be given in reciprocal lattice coordinates: a symbol such as (f, g, h) will mean $\mathbf{k}=f\mathbf{T}_0+g\mathbf{T}_1+h\mathbf{T}_2$ [see Fig. 1(b) for the reciprocal lattice vectors].

The expressions "type A, B, or C" refer to the three cases listed in (vii) of Sec. 4.

$$\Gamma=(000)$$

We find $\mathbf{\Gamma}^{\mathbf{k}}\equiv\mathbf{\Gamma}$, that this point is of type A and that $\mathbf{C}^{\mathbf{k}}=\mathbf{D}_{3h}\times\mathbf{J}$. There is no restriction on $\boldsymbol{\tau}$, which can be any one of the six vectors of this type. For convenience we shall take $\boldsymbol{\tau}=\boldsymbol{\tau}_1$.

$$M=(00\tfrac{1}{2})$$

The condition for $\mathbf{\Gamma}^M$ is $(00\frac{1}{2})$. $(m\mathbf{t}_0+n\mathbf{t}_1+p\mathbf{t}_2)=2\pi\nu$, ($\nu$ integral). Hence:

$$(mnp)\in\mathbf{\Gamma}^M \quad \text{if} \quad p=2\nu, \tag{18}$$

$$(mnp)\in\boldsymbol{\gamma}^M \quad \text{if} \quad p=2\nu+1. \tag{19}$$

The translations of $\boldsymbol{\gamma}^M$ are therefore:

$$\{E\mid m\mathbf{t}_0+n\mathbf{t}_1+(2\nu+1)\mathbf{t}_2\}=\{E\mid m\mathbf{t}_0+n\mathbf{t}_1+2\nu\mathbf{t}_2\}\{E\mid \mathbf{t}_2\}. \tag{20}$$

The first factor in the right-hand side of (20) belongs to $\mathbf{\Gamma}^M$ and can be considered to be the identity. Hence:

$$\boldsymbol{\gamma}^M=\{E\mid\mathbf{0}\}+\{E\mid\mathbf{t}_2\}. \tag{21}$$

The corresponding representatives are 1 and $e^{-i\pi}=-1$.

We find $\mathbf{P}^M\equiv\mathbf{D}_{2h}=\mathbf{C}_{2v}\times\mathbf{C}_i$.

Hence

$$\mathcal{P}^M=\mathbf{C}_{2v}\times\mathbf{J}. \tag{22}$$

This is a group, so that M is of type A.

In (22) we can take

$$\mathbf{J}=\{E\mid\mathbf{0}\}+\{i\mid\boldsymbol{\tau}_1\},$$

and form (15)

$$\mathbf{C}^M=\boldsymbol{\gamma}^M\times(\mathbf{C}_{2v}\times\mathbf{J}). \tag{23}$$

$$K=(0, \bar{1}/3, 2/3)$$

We find:

$$(mnp)\in\mathbf{\Gamma}^K \quad \text{if} \quad 2p-n=3\nu, \quad (\nu \text{ integral}), \tag{24}$$

$$(mnp)\in\boldsymbol{\gamma}^K \quad \text{if} \quad 2p-n=3\nu+1 \quad \text{or} \quad 3\nu+2. \tag{25}$$

In the same manner as for M:

$$\boldsymbol{\gamma}^K=\{E\mid\mathbf{0}\}+\{E\mid\mathbf{t}_1\}+\{E\mid 2\mathbf{t}_1\}, \tag{26}$$

and the corresponding representatives are 1, $\exp(2\pi i/3)$, and $\exp(-2\pi i/3)$, respectively.

$\mathbf{P}^k$ is a $\mathbf{D}_{3h}$ group in which the secondary binary axes and mirror planes are C_{2r}'' and σ_{dr}, respectively ($r=1, 2, 3$). Therefore, in forming $\mathcal{P}^K$, we must associate a translation $\boldsymbol{\tau}$ with these operations.

We take in $\mathcal{P}^K$ the operations $\{C_{2r}''\mid\boldsymbol{\tau}_r\}$ and $\{\sigma_{dr}\mid\boldsymbol{\tau}_r\}$, and we find that $\mathcal{P}^K$ does not close:

$$\{\sigma_{d1}\mid\boldsymbol{\tau}_1\}\{\sigma_{d3}\mid\boldsymbol{\tau}_3\}=\{C_3^-\mid\mathbf{t}_1+\mathbf{t}_2+\mathbf{t}_0\}=\{C_3^-\mid 2\mathbf{t}_1\}. \tag{27}$$

Further multiplication shows that in no case does the product of two operations of $\mathcal{P}^K$ belong to $\boldsymbol{\gamma}^K$: we have a situation of type B. At the same time multiplication shows that $\{C_3^+\mid\mathbf{0}\}$ and $\{C_3^-\mid\mathbf{0}\}$ of $\mathcal{P}^k$ must be replaced by $\{C_3^+\mid\mathbf{t}_1\}$ and $\{C_3^-\mid 2\mathbf{t}_1\}$, respectively (see, e.g., 27), to obtain closure. Also, $\{S_3^+\mid\mathbf{0}\}$ and $\{S_3^-\mid\mathbf{0}\}$ must be replaced by $\{S_3^+\mid\mathbf{t}_1\}$ and $(S_3^-\mid 2\mathbf{t}_1\}$, respectively. These operations, plus the remaining ones of $\mathcal{P}^K$, that require no modification, form the group $\mathcal{P}_t^K$ (see its operations in Table I). From (17)

$$\mathbf{C}^K=\boldsymbol{\gamma}^K\times\mathcal{P}_t^K. \tag{28}$$

As observed in Sec. 4, $\mathcal{P}_t^K$ is isomorphic to $\mathbf{P}^K=\mathbf{D}_{3h}$, so that the representations of $\mathbf{C}^K$ follow at once. The class structure of $\mathcal{P}_t^K$ must, of course, parallel that of $\mathbf{D}_{3h}$, although changes such as the substitution of the class $\{C_3^{\pm}\mid\mathbf{0}\}$ by the class $\{C_3^+\mid\mathbf{t}_1\}$, $\{C_3^-\mid 2\mathbf{t}_1\}$ are required.

The treatment carried out for K is equally valid for $K^*=(0\frac{1}{3}\frac{1}{3})$, except that the right value of $\mathbf{k}$ must be introduced in the representatives $\exp(-i\mathbf{k}\cdot\mathbf{t})$ of the operations of $\boldsymbol{\gamma}^K$ in (28). These representatives are now 1, $\exp(-2\pi i/3)$ and $\exp(2\pi i/3)$, respectively. This remark should serve as a general example of the way in which, if necessary, the representation for points outside our basic domain of the Brillouin zone can be obtained.

$$A=(\tfrac{1}{2}00)$$

The translations of $\mathbf{\Gamma}^A$ are $\{E\mid 2m\mathbf{t}_0+n\mathbf{t}_1+p\mathbf{t}_2\}$ and

$$\boldsymbol{\gamma}^A=\{E\mid\mathbf{0}\}+\{E\mid\mathbf{t}_0\}. \tag{29}$$

$\mathbf{P}^A$ is, as for Γ, $\mathbf{D}_{6h}$ but when we form $\mathcal{P}^A$ we lose the closure. In fact,

$$\{\sigma_d\mid\boldsymbol{\tau}\}\{\sigma_d\mid\boldsymbol{\tau}\}=\{E\mid\mathbf{t}_0\}. \tag{30}$$

We have therefore a group of type C and

$$\mathbf{C}^A=\mathcal{P}^A+\mathcal{P}^A\{E\mid\mathbf{t}_0\}, \tag{31}$$

which, for future reference, can also be written as

$$\mathbf{C}^A=\mathbf{C}^\Gamma+\mathbf{C}^\Gamma\{E\mid\mathbf{t}_0\}. \tag{32}$$

When we consider the class structure of $\mathbf{C}^A$ we shall find that for some operations $\{\alpha\mid\mathbf{w}\}$ and $\{\alpha\mid\mathbf{w}+\mathbf{t}_0\}$ appear in the same class, whereas for others the classes are duplicated when multiplying by $\mathbf{t}_0$. In fact, let us write $\mathbf{D}_{6h}=\mathbf{C}_{3v}\times\mathbf{C}_s\times\mathbf{C}_i$: the operations of $\mathbf{C}_{3v}$ appear in $\mathcal{P}^A$ as $\{\alpha\mid\mathbf{0}\}$ and therefore they still form a subgroup of $\mathbf{C}^A$. Moreover, $\mathbf{C}^A$ will contain $\mathbf{C}_{3v}\times\boldsymbol{\gamma}^A$ as a subgroup and since $\{\sigma_h\mid\mathbf{0}\}$ and $\{i\mid\boldsymbol{\tau}\}$, both of which commute with $\mathbf{C}_{3v}$, cannot introduce additional conjugations, then the classes of $\mathbf{C}_{3v}$ must be duplicated in $\mathbf{C}^A$. On the other hand, the classes of $\mathbf{D}_{6h}$ corresponding to σ_h and i are not duplicated in $\mathbf{C}^A$. In fact, it is easy to prove from (30) that

$$\{\sigma_{d1}\,|\,\boldsymbol{\tau}_1\}^{-1}=\{E\,|\,\mathbf{t}_0\}\{\sigma_{d1}\,|\,\boldsymbol{\tau}_1\},$$

and that therefore the conjugate of $\{\sigma_h\,|\,\mathbf{0}\}$ under $\{\sigma_{d1}\,|\,\boldsymbol{\tau}_1\}$ is $\{\sigma_h\,|\,\mathbf{t}_0\}$. An analogous result is also true for $\{i\,|\,\boldsymbol{\tau}\}$.

It follows from the above that $\mathbf{C}^A$ contains only three new classes with respect to those of $\mathbf{D}_{6h}$, which come from the three original classes of $\mathbf{C}_{3v}$. There are therefore three new representations. It follows from (32) that of the fifteen representations of $\mathbf{C}^A$ the first twelve arise from those of $\mathbf{C}^\Gamma$ by taking the representative of $\{\alpha\,|\,\mathbf{t}_0\}$ equal to that of $\{\alpha\,|\,\mathbf{0}\}$. Since this is equivalent to taking the representative of $\{E\,|\,\mathbf{t}_0\}$ equal to unity, these representations should be discarded [$\exp(-i\mathbf{k}\cdot\mathbf{t}_0)=-1$ for A]. The three extra representations are found by the usual rules to be two 2-dimensional and one 4-dimensional and are given in Sec. 6.

$$L=(\tfrac{1}{2}0\tfrac{1}{2})$$

It can be shown that L and M are related in the same way as A and Γ, so that [cf. (32)]:

$$\mathbf{C}^L=\mathbf{C}^M+\mathbf{C}^M\{E\,|\,\mathbf{t}_0\}, \tag{33}$$

$$\mathcal{P}^L=\mathcal{P}^M=\mathbf{C}_{2v}\times\mathbf{J}. \tag{34}$$

Here $\mathbf{C}_{2v}=\mathbf{C}_2\times\mathbf{C}_s$, where $\mathbf{C}_2=E+C_{21}$, $\mathbf{C}_s=E+\sigma_{v1}$, and it is only the classes of $\mathbf{C}_s$ that split each in two: there are therefore two new classes and two new representations, with respect to $\mathbf{C}^M$, but the representations of $\mathbf{C}^M$ itself should be discarded.

$$H=(1/2,\,\bar{1}/3,\,2/3)$$

We have

$$\mathbf{C}^H=\mathbf{C}^K+\mathbf{C}^K\{E\,|\,\mathbf{t}_0\}. \tag{35}$$

The classes that derive from $\mathbf{C}_3$ are split (as in A) but not those of the remaining operations: this introduces three new irreducible representations.

$$\Delta=(f,\,0,\,0)\qquad 0<f<\tfrac{1}{2}$$

$$\gamma^\Delta=\{E\,|\,m\mathbf{t}_0\},$$

for all m such that mf is not an integer.

$$\mathbf{P}^\Delta=\mathbf{C}_{6v}=\mathbf{C}_{3v}\times\mathbf{C}_2$$

$$\mathcal{P}^\Delta=\mathbf{C}_{3v}\cdot[\{E\,|\,\mathbf{0}\}+\{C_2\,|\,\boldsymbol{\tau}\}]$$

$$\mathbf{C}^\Delta=\gamma^\Delta\cdot\{\mathbf{C}_{3v}\cdot[\{E\,|\,\mathbf{0}\}+\{C_2\,|\,\boldsymbol{\tau}\}]\}. \tag{36}$$

To find the representations we observe that

$$\{C_2\,|\,\boldsymbol{\tau}\}\{C_2\,|\,\boldsymbol{\tau}\}=\{E\,|\,\mathbf{t}_0\}, \tag{37}$$

whence

$$[D\{C_2\,|\,\boldsymbol{\tau}\}]^2=\exp(-i\mathbf{k}\cdot\mathbf{t}_0)\,\mathbf{1} \tag{38}$$

and we can choose

$$D\{C_2\,|\,\boldsymbol{\tau}\}=\pm\exp(-i\mathbf{k}\cdot\mathbf{t}_0/2)\,\mathbf{1}. \tag{39}$$

(36) and (39) show that the representations of $\mathbf{C}^\Delta$ are derived from those of $\mathbf{C}_{3v}$ in accordance with the two possible representatives of $\{C_2\,|\,\boldsymbol{\tau}\}$.

$$U=(f,\,0,\,\tfrac{1}{2})\qquad 0<f<\tfrac{1}{2}$$

$$\mathbf{C}^U=\gamma^U\cdot\{\mathbf{C}_s\cdot[\{E\,|\,\mathbf{0}\}+\{C_2\,|\,\boldsymbol{\tau}\}]\}, \tag{40}$$

where $\mathbf{C}_s=E+\sigma_{v1}$. The representations follow from (40) and (39).

$$P=(f,\,\bar{1}/3,\,2/3)\qquad 0<f<\tfrac{1}{2}$$

$\mathbf{P}^P$ is $\mathbf{C}_{3v}$ and to form $\mathcal{P}^P$ it is enough to take the operations of $\mathcal{P}^K$ that derive from $\mathbf{C}_{3v}$. It is found, in analogy to (38) and (39), that

$$D\{\sigma_{dr}\,|\,\boldsymbol{\tau}_r\}=\pm\exp(-i\mathbf{k}\cdot\mathbf{t}_0/2)\,\mathbf{1},$$

from which value the representations follow easily.

$$\Sigma=(00h)\qquad 0<h<\tfrac{1}{2}$$

Comparing with M (see 23)

$$\mathbf{C}^\Sigma=\gamma^\Sigma\times\mathbf{C}_{2v}.$$

$$T=(0,\,\bar{g},\,2g),\qquad T'=[0,\,\bar{g},\,\tfrac{1}{2}(1+g)]\qquad 0<g<\tfrac{1}{3}$$

$$\mathbf{P}^T=\mathbf{C}_s\times\mathbf{C}_2,\qquad \mathbf{C}_s=E+\sigma_h,\qquad \mathbf{C}_2=E+C_{22}''$$

$$\mathcal{P}^T=[\{E\,|\,\mathbf{0}\}+\{C_{22}''\,|\,\boldsymbol{\tau}_2\}]\times\mathbf{C}_s,$$

which is a group isomorphic to $\mathbf{C}_{2v}$. Also $\mathbf{C}^T=\gamma^T\times\mathcal{P}^T$. For T' substitute $\{C_{21}''\,|\,\boldsymbol{\tau}_1\}$ for $\{C_{22}''\,|\,\boldsymbol{\tau}_2\}$ in the above.

$$R=(\tfrac{1}{2}0h)\qquad 0<h<\tfrac{1}{2}$$

Compare with Σ:

$$C^R=\gamma^R\times\mathbf{C}_{2v}$$

$$S=(\tfrac{1}{2},\,\bar{g},\,2g),\qquad S'=[\tfrac{1}{2},\,\bar{g},\,\tfrac{1}{2}(1+g)],\qquad 0<g<\tfrac{1}{3}$$

$$\mathbf{C}^S=\mathbf{C}^T+\mathbf{C}^T\{E\,|\,\mathbf{t}_0\}.$$

Only the class $\{E\,|\,\mathbf{0}\}$ splits in two: there is one additional representation with respect to those of T. For S' substitute T' for T in the above.

6. RESULTS

The groups $\mathbf{C}^\mathbf{k}$ for all points in the Brillouin zone have been described in Sec. 5 and their character tables are given in Table I. These groups are in most cases isomorphic to well-known point groups and their representations are immediately obtained. As explained in Sec. 5 the groups in question admit in a few cases of some representations that are additional to those of point groups: their characters were obtained from the tables of Herring.[2]

Since we have chosen our axes and notation to coincide with those of Altmann and Bradley[6] we can obtain from their tables, for those groups that are isomorphic to point groups, the irreducible representations in matrix form, although allowance has to be

(*Text continues on p. 40*)

TABLE I. Character tables for the groups of all **k** vectors.

Notes

(*i*) *Points*. The points in **k** space (**k** vectors) should be identified from Fig. 2.

(*ii*) *Symmetry operations*. They are interpreted in the active convention and should be identified from Fig. 1. The suffix r takes the values 1, 2, 3 with reference to the symmetry operations of Fig. 1, and a symbol such as σ_{dr} stands for the three corresponding operations. When more than one translational vector is given in the symbol of an operation, each of the rotational operators indicated must be associated with each of these vectors: $\{\alpha_r \mid \mathbf{u}, \mathbf{v}\}$, for instance, denotes six operations.

When $\boldsymbol{\tau}$ appears without a suffix any of the six vectors of this type (the $\boldsymbol{\tau}_r$ and their reflections in the plane of Fig. 1) can be used.

(*iii*) *Groups and operations*. The groups listed are the groups $\mathbf{C}^{\mathbf{k}}$ defined in the text. They have a translational subgroup $\boldsymbol{\gamma}^{\mathbf{k}}$, the operations of which, and their corresponding characters, are listed at the bottom of the table for each point. Consider a space-group operation given by the product $\{\alpha \mid \mathbf{v}\}\{E \mid \mathbf{t}\}\{E \mid \mathbf{t}'\}$, where $\{\alpha \mid \mathbf{v}\}$ is an operation listed in the first row of the table for each point, and $\{E \mid \mathbf{t}\}$ and $\{E \mid \mathbf{t}'\}$ are a translation of $\boldsymbol{\gamma}^{\mathbf{k}}$ and $\boldsymbol{\Gamma}^{\mathbf{k}}$, respectively. The character of such an operation in the group $\mathbf{G}^{\mathbf{k}}$ is obtained by multiplying the characters of $\{\alpha \mid \mathbf{v}\}$ and $\{E \mid \mathbf{t}\}$ obtained from the body and the bottom of the table respectively by the character of the translation of $\boldsymbol{\Gamma}^{\mathbf{k}}$ which is 1.

It should be noticed that for points on lines of symmetry the translations given for $\boldsymbol{\gamma}^{\mathbf{k}}$ may contain some of $\boldsymbol{\Gamma}^{\mathbf{k}}$ if **k** has fractionary rather than irrational values. This is easily recognized because the characters listed for $\boldsymbol{\gamma}^{\mathbf{k}}$ become unity for certain translations.

(*iv*) *Direct product groups*. In these groups the names of two representations appear in the column under the name of the point. Also, the operations are listed in two complete rows, linked with braces. For the two representations listed together the characters of the operations in the first row are those given in the table. The characters of the operations in the second row are, for the first representation listed, those in the table and, for the second, their negatives.

(*v*) *Representations listed*. Only those representations for which the characters of $\boldsymbol{\gamma}^{\mathbf{k}}$ have the correct value $\exp(-i\mathbf{k}\cdot\mathbf{t})$ are given.

(*vi*) *Nomenclature of the irreducible representations*. This has been chosen so as to coincide as far as possible with the standard notation for the point groups. In particular, whenever $\mathbf{C}^{\mathbf{k}}/\boldsymbol{\gamma}^{\mathbf{k}}$ is isomorphic to a point group, the notation is identical with the standard one, except that for $\mathbf{C}_{2v}$ this has been chosen so as to give priority to σ_h, which is an important operation in the lattice. The main symbols are as follows:

A, B: nondegenerate representations, symmetrical and antisymmetrical, respectively, with respect to C_3^+. (Here and in what follows, the translational part of a symmetry operation, unless stated, will be disregarded.)

$\mathcal{A}$, $\mathcal{B}$: as above, but with respect to C_2', C_2'', or σ_v.

$A^{(2)}$: doubly degenerate representation in which C_3^+ is represented by the matrix $+\mathbf{1}$.

E: doubly degenerate representation in which C_3^+ is not represented by $+\mathbf{1}$.

$\mathcal{E}$: doubly degenerate representation of a group that does not contain C_3^+.

$\mathcal{E}^{(4)}$: four-dimensional representation.

E, E^*: a pair of complex-conjugate two-dimensional representations.

These symbols carry superscripts and suffixes, which denote the behaviour of the representation with respect to certain symmetry elements, as shown below.

Symbol	Position	Operation	Diagonal elements
$'$, $''$	superior	σ_h	± 1
$+$, $-$	inferior	$\{i \mid \boldsymbol{\tau}\}$	± 1
1, 2	inferior	C_2', C_2'', σ_v	± 1
p, m	inferior	$\{C_2 \mid \boldsymbol{\tau}\}$, $\{\sigma_d \mid \boldsymbol{\tau}\}$	$\pm \exp(-i\mathbf{k}\cdot\mathbf{t}_0/2)$

The upper sign in the last column corresponds to the first symbol in the first column. When the main symbol of the representation is $\mathcal{A}$ or $\mathcal{B}$, the suffixes 1 and 2 cannot, of course, be used. The operation to which this suffix refers is chosen as follows: in the nondegenerate representations priority is given to the operations in the order listed. In the degenerate representations σ_v takes priority. As regards the suffixes p, m, $\{C_2 \mid \boldsymbol{\tau}\}$ takes priority over $\{\sigma_d \mid \boldsymbol{\tau}\}$.

For comparison, the number of the representation in Herring's tables is given in brackets on the right of our symbol. To complete the correspondence it is enough to notice that the $+$, $-$ superscripts of Herring coincide with our $+$, $-$ suffixes.

(*vii*) *Time reversal*. In addition to the spatial symmetry operations time reversal must also be considered. This operation introduces additional degeneracies and the criterion given by Herring[8] (see also Elliott[9]) shows that this is the case for R only. There is also time-reversal degeneracy for general points of the top face of the Brillouin zone.

Γ	K	$\{E \mid 0\}$, $\{i \mid \boldsymbol{\tau}\}$ / $\{E \mid 0\}$	$\{C_3^{\pm} \mid 0\}$, $\{S_6^{\mp} \mid \boldsymbol{\tau}\}$, $\{C_3^+ \mid \mathbf{t}_1\}$ / $\{C_3^- \mid 2\mathbf{t}_1\}$	$\{C_{2r}' \mid 0\}$, $\{\sigma_{dr} \mid \boldsymbol{\tau}\}$ / $\{C_{2r}'' \mid \boldsymbol{\tau}_r\}$	$\{\sigma_h \mid 0\}$, $\{C_2 \mid \boldsymbol{\tau}\}$ / $\{\sigma_h \mid 0\}$	$\{S_3^{\pm} \mid 0\}$, $\{C_6^{\mp} \mid \boldsymbol{\tau}\}$, $\{S_3^+ \mid \mathbf{t}_1\}$ / $\{S_3^- \mid 2\mathbf{t}_1\}$	$\{\sigma_{vr} \mid 0\}$, $\{C_{2r}'' \mid \boldsymbol{\tau}\}$ / $\{\sigma_{dr} \mid \boldsymbol{\tau}_r\}$
A_{1+}', A_{1-}' (1, 4)	A_1' (1)	1	1	1	1	1	1
A_{2+}', A_{2-}' (2, 3)	A_2' (3)	1	1	−1	1	1	−1
A_{1+}'', A_{1-}'' (4, 1)	A_1'' (2)	1	1	1	−1	−1	−1
A_{2+}'', A_{2-}'' (3, 2)	A_2'' (4)	1	1	−1	−1	−1	1
E_+', E_-' (5, 6)	E' (5)	2	−1	0	2	−1	0
E_+'', E_-'' (6, 5)	E'' (6)	2	−1	0	−2	1	0

K: $\{E \mid \mathbf{t}_1\}$: $\exp(2\pi i/3)$; $\{E \mid 2\mathbf{t}_1\}$: $\exp(-2\pi i/3)$

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

[9] R. J. Elliott, Phys. Rev. **96**, 266 (1954).

TABLE I (*Continued*)

A	$\{E\mid 0\}$	$\{E\mid t_0\}$	$\{C_3^{\pm}\mid 0\}$	$\{C_3^{\pm}\mid t_0\}$	$\{C_{2r}'\mid 0, t_0\}$	$\{\sigma_h\mid 0, t_0\}$	$\{S_3^{\pm}\mid 0, t_0\}$	$\{\sigma_{vr}\mid 0\}$	$\{\sigma_{vr}\mid t_0\}$
$A_1^{(2)}$ (1)	2	−2	2	−2	0	0	0	2	−2
$A_2^{(2)}$ (2)	2	−2	2	−2	0	0	0	−2	2
$E^{(4)}$ (3)	4	−4	−2	2	0	0	0	0	0

The characters of the operations of A associated with τ:

$$\{i\mid \tau, \tau+t_0\},\quad \{S_6^{\mp}\mid \tau, \tau+t_0\},\quad \{\sigma_{dr}\mid \tau, \tau+t_0\},\quad \{C_2\mid \tau, \tau+t_0\},\quad \{C_6^{\mp}\mid \tau, \tau+t_0\},\quad \{C_{2r}''\mid \tau, \tau+t_0\},$$

vanish in all representations.

L	$\{E\mid 0\}$	$\{E\mid t_0\}$	$\{C_{21}'\mid 0, t_0\}$	$\{\sigma_h\mid 0, t_0\}$	$\{\sigma_{v1}\mid 0\}$	$\{\sigma_{v1}\mid t_0\}$
$\mathcal{E}_1$ (1)	2	−2	0	0	2	−2
$\mathcal{E}_2$ (2)	2	−2	0	0	−2	2

$\{E\mid t_2\}$: −1

The characters of the operations of L that contain τ:

$$\{i\mid \tau_1, \tau_1+t_0\},\quad \{\sigma_{d1}\mid \tau_1, \tau_1+t_0\},\quad \{C_2\mid \tau_1, \tau_1+t_0\},\quad \{C_{21}''\mid \tau_1, \tau_1+t_0\},$$

vanish in both representations.

H	$\{E\mid 0\}$	$\{E\mid t_0\}$	$\{C_3^+\mid t_1\}$ $\{C_3^-\mid 2t_1\}$	$\{C_3^+\mid t_1+t_0\}$ $\{C_3^-\mid 2t_1+t_0\}$	$\{\sigma_h\mid 0, t_0\}$	$\{S_3^+\mid t_1\}$ $\{S_3^-\mid 2t_1+t_0\}$	$\{S_3^+\mid t_1+t_0\}$ $\{S_3^-\mid 2t_1\}$
$A^{(2)}$ (1)	2	−2	2	−2	0	0	0
E (2)	2	−2	−1	−1	0	$-i\sqrt{3}$	$i\sqrt{3}$
E^* (3)	2	−2	−1	−1	0	$i\sqrt{3}$	$-i\sqrt{3}$

$\{E\mid t_1\}$: $\exp(2\pi i/3)$; $\{E\mid 2t_1\}$: $\exp(-2\pi i/3)$

The characters of the operations of H that contain τ:

$$\{C_{2r}'\mid \tau_r, \tau_r+t_0\},\quad \{\sigma_{dr}\mid \tau_r, \tau_r+t_0\},$$

vanish in all representations.

Δ, U, P: $\quad v=\exp(-i\mathbf{k}\cdot t_0/2)$

Δ	$\{E\mid 0\}$	$\{C_3^{\pm}\mid 0\}$	$\{\sigma_{vr}\mid 0\}$	$\{C_2\mid \tau\}$	$\{C_6^{\pm}\mid \tau\}$	$\{\sigma_{dr}\mid \tau\}$
A_{1p} (1)	1	1	1	v	v	v
A_{1m} (2)	1	1	1	$-v$	$-v$	$-v$
A_{2p} (3)	1	1	−1	v	v	$-v$
A_{2m} (4)	1	1	−1	$-v$	$-v$	v
E_p (5)	2	−1	0	$2v$	$-v$	0
E_m (6)	2	−1	0	$-2v$	v	0

$\{E\mid mt_0\}$: $\exp(-im\mathbf{k}\cdot t_0)$

TABLE I (*Continued*)

U	$\{E \mid 0\}$	$\{\sigma_{v1} \mid 0\}$	$\{C_2 \mid \tau_1\}$	$\{\sigma_{d1} \mid \tau_1\}$
$\mathcal{A}_p$ (1)	1	1	v	v
$\mathcal{A}_m$ (2)	1	1	$-v$	$-v$
$\mathcal{B}_p$ (4)	1	-1	v	$-v$
$\mathcal{B}_m$ (3)	1	-1	$-v$	v

$\{E \mid m\mathbf{t}_0\}$: $\exp(-im\mathbf{k}\cdot\mathbf{t}_0)$; $\{E \mid \mathbf{t}_2\}$: -1

P	$\{E \mid 0\}$	$\{C_3^+ \mid \mathbf{t}_1\}$ $\{C_3^- \mid 2\mathbf{t}_1\}$	$\{\sigma_{dr} \mid \tau_r\}$
A_p (1)	1	1	v
A_m (2)	1	1	$-v$
E (3)	2	-1	0

$\{E \mid m\mathbf{t}_0\}$: $\exp(-im\mathbf{k}\cdot\mathbf{t}_0)$; $\{E \mid \mathbf{t}_1\}$: $\exp(2\pi i/3)$; $\{E \mid 2\mathbf{t}_1\}$: $\exp(-2\pi i/3)$

M		$\{E \mid 0\}$, $\{i \mid \tau_1\}$	$\{C_{21}' \mid 0\}$, $\{\sigma_{d1} \mid \tau_1\}$	$\{\sigma_h \mid 0\}$, $\{C_2 \mid \tau_1\}$	$\{\sigma_{v1} \mid 0\}$, $\{C_{21}'' \mid \tau_1\}$
	Σ	$\{E \mid 0\}$	$\{C_{21}' \mid 0\}$	$\{\sigma_h \mid 0\}$	$\{\sigma_{v1} \mid 0\}$
	T	$\{E \mid 0\}$	$\{C_{22}'' \mid \tau_2\}$	$\{\sigma_h \mid 0\}$	$\{\sigma_{d2} \mid \tau_2\}$
	T'	$\{E \mid 0\}$	$\{C_{21}'' \mid \tau_1\}$	$\{\sigma_h \mid 0\}$	$\{\sigma_{d1} \mid \tau_1\}$
	R	$\{E \mid 0\}$	$\{C_{21}' \mid 0\}$	$\{\sigma_h \mid 0\}$	$\{\sigma_{v1} \mid 0\}$
$\mathcal{A}_+'$, $\mathcal{A}_-'$ (1, 2)	$\mathcal{A}'$ (1)	1	1	1	1
$\mathcal{B}_+'$, $\mathcal{B}_-'$ (4, 3)	$\mathcal{B}'$ (4)	1	-1	1	-1
$\mathcal{A}_+''$, $\mathcal{A}_-''$ (2, 1)	$\mathcal{A}''$ (2)	1	1	-1	-1
$\mathcal{B}_+''$, $\mathcal{B}_-''$ (3, 4)	$\mathcal{B}''$ (3)	1	-1	-1	1

M: $\{E \mid \mathbf{t}_2\}$: -1
Σ $\{E \mid p\mathbf{t}_2\}$: $\exp(-ip\mathbf{k}\cdot\mathbf{t}_2)$
T: $\{E \mid n\mathbf{t}_1\}$: $\exp(-in\mathbf{k}\cdot\mathbf{t}_1)$
T': $\{E \mid p\mathbf{t}_2\}$: $\exp(-ip\mathbf{k}\cdot\mathbf{t}_2)$
R: $\{E \mid \mathbf{t}_0\}$: -1; $\{E \mid p\mathbf{t}_2\}$: $\exp(-ip\mathbf{k}\cdot\mathbf{t}_2)$

In R time reversal introduces extra degeneracy: the pairs ($\mathcal{A}'$, $\mathcal{B}''$) and ($\mathcal{B}'$, $\mathcal{A}''$) become degenerate.

S S'	$\{E \mid 0\}$ $\{E \mid 0\}$	$\{E \mid \mathbf{t}_0\}$ $\{E \mid \mathbf{t}_0\}$	$\{C_{22}'' \mid \tau_2, \tau_2+\mathbf{t}_0\}$ $\{C_{21}'' \mid \tau_1, \tau_1+\mathbf{t}_0\}$	$\{\sigma_h \mid 0, \mathbf{t}_0\}$ $\{\sigma_h \mid 0, \mathbf{t}_0\}$	$\{\sigma_{d2} \mid \tau_2, \tau_2+\mathbf{t}_0\}$ $\{\sigma_{d1} \mid \tau_1, \tau_1+\mathbf{t}_0\}$
$\mathcal{E}$ (1)	2	-2	0	0	0

S: $\{E \mid n\mathbf{t}_1\}$: $\exp(-in\mathbf{k}\cdot\mathbf{t}_1)$

S': $\{E \mid p\mathbf{t}_2\}$: $\exp(-ip\mathbf{k}\cdot\mathbf{t}_2)$

made for the change from the passive to the active interpretation of the operators. In the remaining cases the matrices were not difficult to obtain, by an extension of the methods used for the point groups. The matrix representations are listed in Table II. In Table III we give the compatibilities between the irreducible representations as $\mathbf{k}$ moves over the Brillouin zone. The lattice harmonics are tabulated in Table IV.

(*Text continues on p. 45*)

TABLE II. The multidimensional representations.

Notes

See notes (*i*), (*ii*), (*iii*), and (*v*) to Table I.

(*i*) *Key to the symbols.* In the body of the table Greek letters are matrices and Latin letters complex numbers (i here should not be confused with the symbol for the inversion). The matrices $\epsilon, \alpha, \beta, \lambda, \mu, \nu, \kappa, \rho$ are as defined in I, Table III(a). The (2×2) matrix ω is defined below. All primed Greek letters are diagonal supermatrices, the diagonal elements of which are the unprimed (2×2) matrices, both of them positive for singly primed symbols, the first positive and the second negative for doubly primed symbols. As an example, we define α' and α'' below. η is a 4×4 matrix defined below in supermatrix notation.

$$\omega = \begin{bmatrix} w & \\ & w^* \end{bmatrix} \quad \alpha' = \begin{bmatrix} \alpha & \\ & \alpha \end{bmatrix} \quad \alpha'' = \begin{bmatrix} \alpha & \\ & -\alpha \end{bmatrix} \quad \eta = \begin{bmatrix} & -\epsilon \\ -\epsilon & \end{bmatrix}$$

$$v = \exp(-i\mathbf{k}\cdot\mathbf{t}_0/2) \qquad w = \exp(2\pi i/3)$$

(*ii*) *Matrices for the space-group operations.* The complete form of the space-group operation should be read off Table I: consider an operation $\{\alpha \mid \mathbf{v}\}\{E \mid \mathbf{t}\}$, where $\{E \mid \mathbf{t}\}\epsilon\gamma^{\mathbf{k}}$. Disregard $\mathbf{v}$, unless it includes $\mathbf{t}_0$. Obtain the matrices from the present table in the row corresponding to α. If $\mathbf{v}$ includes $\mathbf{t}_0$ multiply this matrix by -1 (where $\mathbf{1}$ is the unit matrix of appropriate dimension). The matrix for $\{E \mid \mathbf{t}\}$ is obtained by multiplying the character listed for $\{E \mid \mathbf{t}\}$ in Table I by $\mathbf{1}$.

	Γ				K		A			L		H			Δ		P	S	S′
	E_+'	E_-'	E_+''	E_-''	E'	E''	$A_1^{(2)}$	$A_2^{(2)}$	$E^{(4)}$	$\mathcal{E}_1$	$\mathcal{E}_2$	$A^{(2)}$	E	E^*	E_p	E_m	E	$\mathcal{E}$	$\mathcal{E}$
E	ϵ	ϵ	ϵ	ϵ	ϵ	ϵ	ϵ	ϵ	ϵ'	ϵ	ϵ	ϵ	ϵ	ϵ	ϵ	ϵ	ϵ	ϵ	ϵ
C_3^+	β	β	β	β	β	β	ϵ	ϵ	β'			ϵ	ω^*	ω^*	β	β	β		
C_3^-	α	α	α	α	α	α	ϵ	ϵ	α'			ϵ	ω	ω	α	α	α		
C_{21}'	λ	λ	$\bar\lambda$	$\bar\lambda$			λ	$\bar\lambda$	λ''	λ	$\bar\lambda$								
C_{22}'	μ	μ	$\bar\mu$	$\bar\mu$			λ	$\bar\lambda$	μ''										
C_{23}'	ν	ν	$\bar\nu$	$\bar\nu$			λ	$\bar\lambda$	ν''										
σ_h	ϵ	ϵ	$\bar\epsilon$	$\bar\epsilon$	ϵ	$\bar\epsilon$	λ	λ	ϵ''	λ	λ	λ	λ	$\bar\lambda$				λ	λ
S_3^+	β	β	$\bar\beta$	$\bar\beta$	β	$\bar\beta$	λ	λ	β''			λ	$\lambda\omega^*$	$\bar\lambda\omega^*$					
S_3^-	α	α	$\bar\alpha$	$\bar\alpha$	α	$\bar\alpha$	λ	λ	α''			λ	$\lambda\omega$	$\bar\lambda\omega$					
σ_{v1}	λ	λ	λ	λ			ϵ	$\bar\epsilon$	λ'	ϵ	$\bar\epsilon$				λ	λ			
σ_{v2}	μ	μ	μ	μ			ϵ	$\bar\epsilon$	μ'						μ	μ			
σ_{v3}	ν	ν	ν	ν			ϵ	$\bar\epsilon$	ν'						ν	ν			
i	ϵ	$\bar\epsilon$	ϵ	$\bar\epsilon$			$i\bar\rho$	$i\rho$	$\eta\epsilon'$	$i\bar\rho$	$i\rho$								
S_6^-	β	$\bar\beta$	β	$\bar\beta$			$i\bar\rho$	$i\rho$	$\eta\beta'$										
S_6^+	α	$\bar\alpha$	α	$\bar\alpha$			$i\bar\rho$	$i\rho$	$\eta\alpha'$										
σ_{d1}	λ	$\bar\lambda$	$\bar\lambda$	λ	λ	$\bar\lambda$	$i\kappa$	$i\kappa$	$\eta\lambda''$	$i\kappa$	$i\kappa$	$i\kappa$	$i\bar\kappa$	$i\bar\kappa$	$v\lambda$	$v\bar\lambda$	$v\lambda$		$i\kappa$
σ_{d2}	μ	$\bar\mu$	$\bar\mu$	μ	μ	$\bar\mu$	$i\kappa$	$i\kappa$	$\eta\mu''$			$i\kappa$	$i\bar\kappa\omega^*$	$i\bar\kappa\omega^*$	$v\mu$	$v\bar\mu$	$v\mu$	$i\kappa$	
σ_{d3}	ν	$\bar\nu$	$\bar\nu$	ν	ν	$\bar\nu$	$i\kappa$	$i\kappa$	$\eta\nu''$			$i\kappa$	$i\bar\kappa\omega$	$i\bar\kappa\omega$	$v\nu$	$v\bar\nu$	$v\nu$		
C_2	ϵ	$\bar\epsilon$	$\bar\epsilon$	ϵ			$i\kappa$	$i\bar\kappa$	$\eta\epsilon''$	$i\kappa$	$i\bar\kappa$				$v\epsilon$	$v\bar\epsilon$			
C_6^-	β	$\bar\beta$	$\bar\beta$	β			$i\kappa$	$i\bar\kappa$	$\eta\beta''$						$v\beta$	$v\bar\beta$			
C_6^+	α	$\bar\alpha$	$\bar\alpha$	α			$i\kappa$	$i\bar\kappa$	$\eta\alpha''$						$v\alpha$	$\bar\alpha$			
C_{21}''	λ	$\bar\lambda$	λ	$\bar\lambda$	λ	λ	$i\bar\rho$	$i\bar\rho$	$\eta\lambda'$	$i\bar\rho$	$i\bar\rho$	$i\bar\rho$	$i\rho$	$i\bar\rho$					$i\bar\rho$
C_{22}''	μ	$\bar\mu$	μ	$\bar\mu$	μ	μ	$i\bar\rho$	$i\bar\rho$	$\eta\mu'$			$i\bar\rho$	$i\rho\omega^*$	$i\bar\rho\omega^*$				$i\bar\rho$	
C_{23}''	ν	$\bar\nu$	ν	$\bar\nu$	ν	ν	$i\bar\rho$	$i\bar\rho$	$\eta\nu'$			$i\bar\rho$	$i\rho\omega$	$i\bar\rho\omega$					

TABLE III. Compatibilities for all the representations of $\mathbf{D}_{6h}{}^4$.

Notes

(*i*) *Compatibilities* for the irreducible representations along the seven lines of symmetry are given. (Along the lines ASH and $LS'H$ all the representations are compatible.) To consider any circuit several of these lines must be combined.

(*ii*) All the representations listed in one column of a block corresponding to a symmetry line are compatible. When more than one sign is given either of them can be used.

Γ	$A_{1\pm}'$, $E_{\pm}'$	$A_{2\pm}'$, $E_{\pm}'$	$A_{1\pm}''$, $E_{\pm}''$	$A_{2\pm}''$, $E_{\pm}''$		
Σ	$\mathcal{A}'$	$\mathcal{B}'$	$\mathcal{A}''$	$\mathcal{B}''$		
M	$\mathcal{A}_{\pm}'$	$\mathcal{B}_{\pm}'$	$\mathcal{A}_{\pm}''$	$\mathcal{B}_{\pm}''$		
Γ	A_{1+}', A_{2-}''	A_{1-}', A_{2+}''	A_{2+}', A_{1-}''	A_{2-}', A_{1+}''	E_{+}', E_{-}''	E_{-}', E_{+}''
Δ	A_{1p}	A_{1m}	A_{2p}	A_{2m}	E_p	E_m
A	$A_1^{(2)}$	$A_1^{(2)}$	$A_2^{(2)}$	$A_2^{(2)}$	$E^{(4)}$	$E^{(4)}$
Γ	A_{1+}', A_{2-}', $E_{\pm}'$	A_{2+}', A_{1-}', $E_{\pm}'$	A_{1-}'', A_{2+}'', $E_{\pm}''$	A_{1+}'', A_{2-}'', $E_{\pm}''$		
T	$\mathcal{A}'$	$\mathcal{B}'$	$\mathcal{A}''$	$\mathcal{B}''$		
K	A_1', E'	A_2', E'	A_1'', E''	A_2'', E''		
M	$\mathcal{A}_{+}'$, $\mathcal{B}_{-}'$	$\mathcal{A}_{-}'$, $\mathcal{B}_{+}'$	$\mathcal{A}_{-}''$, $\mathcal{B}_{+}''$	$\mathcal{A}_{+}''$, $\mathcal{B}_{-}''$		
T'	$\mathcal{A}'$	$\mathcal{B}'$	$\mathcal{A}''$	$\mathcal{B}''$		
K	A_1', E'	A_2', E'	A_1'', E''	A_2'', E''		
M	$\mathcal{A}_{+}'$, $\mathcal{B}_{-}''$	$\mathcal{A}_{-}'$, $\mathcal{B}_{+}''$	$\mathcal{B}_{+}'$, $\mathcal{A}_{-}''$	$\mathcal{B}_{-}'$, $\mathcal{A}_{+}''$		
U	$\mathcal{A}_p$	$\mathcal{A}_m$	$\mathcal{B}_p$	$\mathcal{B}_m$		
L	$\mathcal{E}_1$	$\mathcal{E}_1$	$\mathcal{E}_2$	$\mathcal{E}_2$		
K	A_1', A_2''	A_2', A_1''	E', E''			
P	A_p	A_m	E			
H	$A^{(2)}$	$A^{(2)}$	E, E^*			
A	$A_1^{(2)}$, $E^{(4)}$	$A_2^{(2)}$, $E^{(4)}$	$A_2^{(2)}$, $E^{(4)}$	$A_1^{(2)}$, $E^{(4)}$		
R	$\mathcal{A}'$	$\mathcal{B}'$	$\mathcal{A}''$	$\mathcal{B}''$		
L	$\mathcal{E}_1$	$\mathcal{E}_2$	$\mathcal{E}_2$	$\mathcal{E}_1$		

TABLE IV. The lattice harmonics for the hexagonal close-packed lattice.

Notes

(*i*) *Representations.* The representations spanned by the bases given here are obtained from Table I (one dimensional) and Table II (two and four dimensional). These representations correspond to active operators.

(*ii*) *Periodic extension.* The expansions are given in a centered unit cell. This contains two halves one around the atom at the origin in Fig. 1 and the other around either the atom at $\boldsymbol{\tau}_1$ or the one at $\boldsymbol{\tau}_2$. The expansions outside this unit cell are obtained by application of the Bloch theorem (see I.5).

(*iii*) *Values of l and m.* l is given mod $(+2)$, that is any multiple of 2 can be added to the value of l in the table. m is given either mod $(+s)$, with an analogous meaning or mod s in which case a multiple of s can be added to or subtracted from the value of m in the table. An indication for this is given in the last column of the table. l and m appear in a double column and the permitted values are obtained by forming the whole succession derived from the two pairs given. For instance, for $\Gamma A_{1+}''$ or $\Gamma A_{1-}''$, the permitted values of l and m are: (4, 3), (6, 3), (7, 6), (8, 3), (9, 6), (10, 3), (10, 9), (11, 6), etc.

(*iv*) *The $\pm$ sign.* When there are two representatives listed in the same row, the upper sign in the harmonics expansion corresponds to the first of the two representations.

(*v*) *The spherical harmonics.* We use the following notation for them:

$$m = Y_l^m(\theta,\phi); \qquad (-m) = Y_l^{-m}(\theta,\phi);$$

$$c = Y_l^{m,c}(\theta,\phi); \qquad s = Y_l^{m,s}(\theta,\phi);$$

where the harmonics themselves are defined in I (11), (12), and (13).

The four symbols above correspond to harmonics centered at the origin with a set of axes x, y, z shown in Fig. 1. Harmonics centered around the second atom in a set of axes inverted with respect of $x\ y\ z$ are denoted by placing a bar — above any of the four symbols (atom at $\boldsymbol{\tau}_1$) or a tilde $\sim$ (atom at $\boldsymbol{\tau}_2$).

(*vi*) *The expansions.* They are obtained from the column headed "harmonics" by associating with the harmonics listed there any of the values of l and m permitted. They are normally given in one line but for R the harmonic around each center must be read from a separate line and the appropriate combination formed as indicated in the table. In most cases the harmonic around the second center carries a coefficient ± 1. In others, coefficients with the following values are used:

$q\ = \exp(\pi i f)$ ($f = \mathbf{T}_0$ component of the $\mathbf{k}$ vector),

$r\ = \exp(2\pi i/6)$,

x, y = arbitrary coefficients.

In the nondegenerate representations only one expansion is usually given in each line. If there are two separated by "or" it

TABLE IV (*Continued*)

means that either of them can be used. In degenerate representations all the partners in one basis are given in one line. The expansions given in this table are two-center expansions, symmetry-adapted over the unit cell. To obtain the full lattice harmonics combinations of them over all lattice points must be obtained with the appropriate Bloch coefficients, as in (I.5).

(*vii*) *Bases.* They are understood as *row* vectors. Their transformation properties are obtained by postmultiplying them with the matrix representative.

(*viii*) *An example of the use of the table.* The following are suitable bases for $HA^{(2)}$:

$$(Y_1^1, -i\bar{Y}_1^{-1}), \quad (i\bar{Y}_2^{-1}, Y_2^1), \quad (Y_2^{-2}, -i\bar{Y}_2^2),$$
$$(Y_3^1, -i\bar{Y}_3^{-1}), \quad (i\bar{Y}_3^2, Y_3^{-2}), \quad (i\bar{Y}_4^{-1}, Y_4^1),$$
$$(Y_4^{-2}, -i\bar{Y}_4^2), \quad (Y_4^4, -i\bar{Y}_4^{-4}), \quad \text{etc.}$$

An expansion for the first column of the representation around the atom at the origin will be

$$A_1R_1^1(r)\,Y_1^1(\theta,\phi)+A_2R_2^{-2}(r)\,Y_2^{-2}(\theta,\phi)+A_3R_3^1(r)\,Y_3^1(\theta,\phi)$$
$$+A_{4,-2}R_4^{-2}(r)\,Y_4^{-2}(\theta,\phi)+A_{4,4}R_4^4(r)\,Y_4^4(\theta,\phi)+\cdots,$$

and the corresponding expansion for the atom at τ_1 will be:

$$B_2\bar{R}_2^{-1}(r)\,\bar{Y}_2^{-1}(\theta,\phi)+B_3\bar{R}_3^2(r)\,\bar{Y}_3^2(\theta,\phi)$$
$$+B_4\bar{R}_4^{-1}(r)\,\bar{Y}_4^{-1}(\theta,\phi)+\cdots.$$

Here the A's and B's are arbitrary complex coefficients in a convenient notation and the R's and $\bar{R}$'s are arbitrary radial functions around the first and second atom, respectively.

		l	m	l	m	Harmonics	m
Γ	A_{1+}', A_{1-}'	0	0	3	3	$c\pm\bar{c}$	mod (+6)
	A_{2+}', A_{2-}'	3	3	6	6	$s\pm\bar{s}$	
	A_{1+}'', A_{1-}''	4	3	7	6	$s\pm\bar{s}$	
	A_{2+}'', A_{2-}''	1	0	4	3	$c\pm\bar{c}$	
	E_+', E_-'	1	1	4	4	$c\pm\bar{c}$, $s\pm\bar{s}$	
		2	2	5	5	$c\pm\bar{c}$, $-(s\pm\bar{s})$	
	E_+'', E_-''	2	1	5	4	$c\pm\bar{c}$, $s\pm\bar{s}$	
		3	2	6	5	$c\pm\bar{c}$, $-(s\pm\bar{s})$	
M	$\mathcal{A}_+'$, $\mathcal{A}_-'$	0	0	1	1	$c\pm\bar{c}$	mod (+2)
	$\mathcal{B}_+'$, $\mathcal{B}_-'$	1	1	2	2	$s\pm\bar{s}$	
	$\mathcal{A}_+''$, $\mathcal{A}_-''$	2	1	3	2	$s\pm\bar{s}$	
	$\mathcal{B}_+''$, $\mathcal{B}_-''$	1	0	2	1	$c\pm\bar{c}$	
K	A_1', A_2'	1	1	4	4	$m\pm(-\bar{m})$	mod 6
	A_1'', A_2''	2	1	5	4	$m\pm(-\bar{m})$	
	E'	0	0	3	3	$m+(-\bar{m})$, $i[m-(-\bar{m})]$	
		2	2	5	5	$m+(-\bar{m})$, $-i[m-(-\bar{m})]$	
	E''	1	0	4	3	$m-(-\bar{m})$, $i[m+(-\bar{m})]$	
		3	2	6	5	$m-(-\bar{m})$, $-i[m+(-\bar{m})]$	
A	$A_1^{(2)}$	0	0	3	3	c, $-i\bar{c}$	mod (+6)
		1	0	4	3	$\bar{c}$, $-ic$	
	$A_2^{(2)}$	3	3	6	6	s, $i\bar{s}$	
		4	3	7	6	$\bar{s}$, is	
	$E^{(4)}$	1	1	4	4	c, s, $-\bar{c}$, $-\bar{s}$	
		2	2	5	5	c, $-s$, $-\bar{c}$, $\bar{s}$	
		2	1	5	4	$\bar{c}$, $\bar{s}$, $-c$, $-s$	
		3	2	6	5	$\bar{c}$, $-\bar{s}$, $-c$, s	
L	$\mathcal{E}_1$	0	0	1	1	c, $-i\bar{c}$	mod (+2)
		1	0	2	1	$\bar{c}$, $-ic$	
	$\mathcal{E}_2$	1	1	2	2	s, $i\bar{s}$	
		2	1	3	2	$\bar{s}$, is	
H	$A^{(2)}$	1	1	4	4	m, $-i(-\bar{m})$	mod 6
		2	1	5	4	$i(-\bar{m})$, m	
	E	2	2	5	5	m, $i(-\bar{m})$	
		1	0	4	3	$-i(-\bar{m})$, m	
	E^*	0	0	3	3	$i(-\bar{m})$, m	
		3	2	6	5	m, $-i(-\bar{m})$	

TABLE IV (*Continued*)

		l	m	l	m	Harmonics	m
Δ	A_{1p}, A_{1m}	0	0	3	3	$c\pm q\bar{c}$	mod (+6)
		1	0	4	3	$c\mp q\bar{c}$	
	A_{2p}, A_{2m}	3	3	6	6	$s\pm q\bar{s}$	
		4	3	7	6	$s\mp q\bar{s}$	
	E_p, E_m	1	1	4	4	$c\pm q\bar{c}$, $s\pm q\bar{s}$	
		2	2	5	5	$c\pm q\bar{c}$, $-(s\pm q\bar{s})$	
		2	1	5	4	$c\mp q\bar{c}$, $s\mp q\bar{s}$	
		3	2	6	5	$c\mp q\bar{c}$, $-(s\mp q\bar{s})$	
U	$\mathcal{A}_p$, $\mathcal{A}_m$	0	0	1	1	$c\pm q\bar{c}$	mod (+2)
		1	0	2	1	$c\mp q\bar{c}$	
	$\mathcal{B}_p$, $\mathcal{B}_m$	1	1	2	2	$s\pm q\bar{s}$	
		2	1	3	2	$s\mp q\bar{s}$	
P	A_p, A_m	1	1	4	4	$m\pm q(-\bar{m})$	mod 6
		2	1	5	4	$m\mp q(-\bar{m})$	
	E	0	0	3	3	$m+q(-\bar{m})$, $\mathrm{i}[m-q(-\bar{m})]$	
		2	2	5	5	$m+q(-\bar{m})$, $-\mathrm{i}[m-q(-\bar{m})]$	
		1	0	4	3	$m-q(-\bar{m})$, $\mathrm{i}[m+q(-\bar{m})]$	
		3	2	6	5	$m-q(-\bar{m})$, $-\mathrm{i}[m+q(-\bar{m})]$	
Σ	$\mathcal{A}'$	0	0	1	1	$xc+y\bar{c}$	mod (+2)
	$\mathcal{B}'$	1	1	2	2	$xs+y\bar{s}$	
	$\mathcal{A}''$	2	1	3	2	$xs+y\bar{s}$	
	$\mathcal{B}''$	1	0	2	1	$xc+y\bar{c}$	
T	$\mathcal{A}'$, $\mathcal{B}'$	0	0	3	3	$c\pm\tilde{c}$	mod (+6)
		3	3	6	6	$s\mp\tilde{s}$	
		1	1	4	4	$c\mp[\frac{1}{2}\tilde{c}+(\sqrt{3}/2)\tilde{s}]$	
		1	1	4	4	$s\pm[\frac{1}{2}\tilde{s}-(\sqrt{3}/2)\tilde{c}]$	
		2	2	5	5	$c\mp[\frac{1}{2}\tilde{c}-(\sqrt{3}/2)\tilde{s}]$	
		2	2	5	5	$s\pm[\frac{1}{2}\tilde{s}+(\sqrt{3}/2)\tilde{c}]$	
	$\mathcal{A}''$, $\mathcal{B}''$	1	0	4	3	$c\pm\tilde{c}$	
		4	3	7	6	$s\mp\tilde{s}$	
		2	1	5	4	$c\mp[\frac{1}{2}\tilde{c}+(\sqrt{3}/2)\tilde{s}]$	
		2	1	5	4	$s\pm[\frac{1}{2}\tilde{s}-(\sqrt{3}/2)\tilde{c}]$	
		3	2	6	5	$c\mp[\frac{1}{2}\tilde{c}-(\sqrt{3}/2)\tilde{s}]$	
		3	2	6	5	$s\pm[\frac{1}{2}\tilde{s}+(\sqrt{3}/2)\tilde{c}]$	
T'	$\mathcal{A}'$, $\mathcal{B}'$	0	0	1	1	$c\pm\bar{c}$ or $s\mp\bar{s}$	mod (+2)
	$\mathcal{A}''$, $\mathcal{B}''$	1	0	2	1	$c\pm\bar{c}$ or $s\mp\bar{s}$	
R	$\mathcal{A}'$	0	0	1	1	$xc+$	mod (+2)
		1	0	2	1	$y\bar{c}$.	
	$\mathcal{B}'$	1	1	2	2	$xs+$	
		2	1	3	2	$y\bar{s}$.	
	$\mathcal{A}''$	2	1	3	2	$xs+$	
		1	1	2	2	$y\bar{s}$.	
	$\mathcal{B}''$	1	0	2	1	$xc+$	
		0	0	1	1	$y\bar{c}$.	
S	$\mathcal{E}$	0	0	3	3	m, $-\mathrm{i}(-\tilde{m})$	mod 6
		1	0	4	3	$\mathrm{i}(-\tilde{m})$, m	
		1	1	4	4	m, $\mathrm{i}r(-\tilde{m})$	
		2	1	5	4	$-\mathrm{i}r(-\tilde{m})$, m	
		2	2	5	5	m, $\mathrm{i}r^*(-\tilde{m})$	
		3	2	6	5	$-\mathrm{i}r^*(-\tilde{m})$, m	
S'	$\mathcal{E}$	0	0	1	1	m, $-\mathrm{i}(-\bar{m})$	mod 2
		1	0	2	1	$\mathrm{i}(-\bar{m})$, m	

ACKNOWLEDGMENT

This work was supported by a grant from the U.K.A.E.A. which is gratefully acknowledged.

Note added in proof. Since this paper was communicated we have learned that a paper by Professor J. C. Slater on the same subject will appear in the same issue. Professor Slater proposes in his paper a new scheme of definitions for the function-space operators and since this is different from the one that we have used, we feel that a few comments are necessary.

We shall try to enunciate explicitly the conventions which we believe are used by Professor Slater. In doing so, we shall drop the translational part of the space-group operators, since the new features of Professor Slater's scheme do not depend on them. A point group operator R is now defined, from Slater's Eqs. (5) and (6) as

$$Rf(\mathbf{r})=f(\alpha\mathbf{r}). \qquad (41)$$

However, this equation appears to be valid *only when the variable* is $\mathbf{r}$. For instance, if we introduce a new variable

$$\mathbf{s}=\mathbf{g}(\mathbf{r}) \qquad (42)$$

then,

$$Rf(\mathbf{s})\neq f(\alpha\mathbf{s}). \qquad (43)$$

Rather, it seems to us that Professor Slater defines

$$Rf(\mathbf{s})=Rf[\mathbf{g}(\mathbf{r})]=f[\mathbf{g}(\alpha\mathbf{r}]. \qquad (44)$$

In this way he maintains the isomorphism of his operators as follows: Take

$$R_iR_j=R_k \qquad (45)$$

and

$$\alpha^j\alpha^i=\alpha^k. \qquad (46)$$

[Cf. Slater's Eq. (11) and the line above it.] Then, form

$$R_jf(\mathbf{r})=f(\alpha^j\mathbf{r}). \qquad (47)$$

Operating with R_i on both sides of this equation, we have

$$R_iR_jf(\mathbf{r})=R_if(\alpha^j\mathbf{r}), \qquad (48)$$

which, on using (44), gives

$$R_iR_jf(\mathbf{r})=f(\alpha^j\alpha^i\mathbf{r}). \qquad (49)$$

Now, (45) and (46) substituted in (49) give the correct result

$$R_kf(\mathbf{r})=f(\alpha^k\mathbf{r}). \qquad (50)$$

It is seen that the procedure given from (47) to (50) parallels that given by Wigner[10] in the English edition of his book (p. 106) as an example of a wrong modus operandi. In particular, with the ordinary function-space operators as defined for instance by Wigner, the step in italics under our Eq. (47) is not valid: these operators operate on functions and (47) is a numerical, not a functional, relation. (It states that the *value* of the function R_jf at the point $\mathbf{r}$ is equal to the *value* of the function f at the point $\alpha^j\mathbf{r}$). In fairness to Professor Slater it should be said that Wigner's criticism could be considered irrelevant in the new scheme, since, on account of (43), *Slater's operators are no longer defined as operators that transform functions and should be considered as formal entities defined by* (41) *and* (44).

In fact, we believe that Professor Slater may be consistent, but this is at the expense of a very substantial price. The whole theory of linear transformations is based on the fact that (43) and (41) are equally valid. Also, the meaning of the operators R in the usual scheme is clear and perfectly well defined, whereas we have seen that in the new scheme they have to be treated as *ad-hoc* entities for which it cannot even be claimed that they transform functions. The reader must appreciate, for instance, that Slater's inversion applied on exp (s) may not give the function exp ($-s$).

The Slater operator is an entirely new symbol, tied up to one *absolute* system of axes (his $\mathbf{r}$ variable) and again this is contrary to the mathematical practice of the last century where linear transformations are always defined with respect to floating systems of axes.

One of us (C. J. B.) would like to acknowledge correspondence with Professor Slater and the other a kind letter from Professor Wigner in 1954 that set him on the right path after his early mistakes in this field.

[10] E. P. Wigner, *Group Theory* (Academic Press Inc., New York, 1959).