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

The Crystallographic Point Groups as Semi-Direct Products

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Phil. Trans. R. Soc. Lond. A 1963 **255**, 216-240
doi: 10.1098/rsta.1963.0003

THE CRYSTALLOGRAPHIC POINT GROUPS AS SEMI-DIRECT PRODUCTS

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(*Communicated by W. Hume-Rothery, F.R.S.—Received* 18 *December* 1961)

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This paper aims at providing a systematic treatment of the crystallographic point groups. Some well-known properties of them, in terms of the theory of the poles of finite rotations, are first discussed, so as to provide a simple way for recognizing their invariant subgroups. A definition of the semi-direct product is then given, and it is shown that all crystallographic point groups can be expressed as a semi-direct product of one of their invariant subgroups by a cyclic subgroup. Many useful relations between point groups can be obtained by exploiting the properties of the triple and mixed triple semi-direct products, which are defined.

Much of the rest of the paper is devoted to the theory of the representations of semi-direct products. The treatment here parallels that given by Seitz (1936) for the reduction of space groups in terms of the representations of its invariant subgroups (the translation groups). The latter, however, are always Abelian and this is not always the case for point groups. The full treatment of the general case, such as given by McIntosh (1958), is laborious and it is shown that, if the emphasis is placed on the bases of the representations, rather than the representations themselves, it is possible to achieve the reduction of the point groups by a method hardly more involved than that required when the invariant subgroup is Abelian.

It is also shown that, just as for space groups, the representations of the invariant subgroups can be denoted and visualized by means of a vector, which allows a very rapid classification of the representations, very much as the **k** vector as used by Bouckaert, Smoluchowski & Wigner (1936) allows the formalism of the Seitz method for space groups to be carried out in a graphical fashion.

One of the major consequences of this work is that it affords a substantial simplification in the use of the symmetrizing and projection operators that are required to obtain symmetry-adapted functions: a very systematic alternative to the method given by Melvin (1956) is therefore provided.

In the last section of the paper all the techniques discussed are applied in detail, as an example, to the cubic groups. The projection operators are used to obtain symmetry-adapted spherical harmonics for these groups.

The paper might be found useful as an introduction to the methods for the reduction of space groups.

1. Introduction

One of the major problems in the study of the symmetries of the point groups consists in the derivation of functions that belong to the irreducible representations of these groups, which we shall call, following Melvin (1956), symmetry-adapted functions. In order to do this one must use some well-known symmetrizing or projection operators which will be described later on in this paper. When the functions in question are spherical harmonics—which are required in a variety of problems such as cellular calculations in metals or the study of molecular hybrids—the application of these operators to the point groups can be done in a systematic and simple fashion, as shown by Altmann (1957*a*). Nevertheless, the use of the symmetrizing operators can be rather tiresome in the more general cases and Melvin (1956) gave a method to simplify the work. Melvin's method, however, is largely empirical, being based on some observed features of the representations. Accordingly, Altmann (1957*b*) suggested a more systematic procedure, based on the application of the method first used by Seitz (1936) and further developed by Bouckaert *et al.* (1936) for the reduction of space groups. The possibility of this application arises from the fact that all crystallographic point groups admit of an invariant subgroup which is either cyclic or a direct product of cyclic groups. This can therefore take the place of the translation group in Seitz's theory and, just as for the space groups, the irreducible representations of the group can be generated in terms of the irreducible representations of its invariant subgroup. Of course, to accomplish this task would appear to be a problem of mere academic interest, because the reduction of the point groups is a fully solved problem. Nevertheless, when it is carried out by the method suggested, it is found that a considerable simplification can be obtained in the handling of the symmetrizing operators. Therefore, following the above-mentioned suggestion, McIntosh (1960) remarked that the above procedure is tantamount to expressing the point groups as semi-direct products, as introduced by Mackey (1949, 1952). In fact, Mackey and others (see Lomont 1959, chapter V) have given a number of powerful theorems for the reduction of semi-direct products. The advantage of this approach, over the one originally suggested by the present author lies in the fact that the semi-direct product theory can be used for invariant subgroups which are not Abelian: the theory given by Seitz provided only for Abelian subgroups, since the translation subgroup of a space group always satisfies this condition. Accordingly, McIntosh (1958, 1960) developed in detail the theory of the reduction of the semi-direct products. However, McIntosh constructed his theory starting from the matrix representations and going from them to the corresponding bases. We shall show in this paper that if this approach is reversed one obtains a formalism that is much easier to use. We do not propose in this paper to provide an exhaustive treatment of the semi-direct products, as this can be obtained from the references given. Rather, we want to use the theory very much as Bouckaert *et al.* (1936) used Seitz's theory, to provide a formalism that is both graphical and extremely easy to use. Nevertheless, we shall give in § 5 some formal proofs of such parts of the theory as are required to put our formalism on a sure footing.

It should be noticed that irrespective of its use in the derivation of symmetry-adapted functions, the semi-direct product theory of the point groups affords the most systematic approach to their study and it is therefore a valuable tool on its own. It is extremely useful in particular in bringing out clearly the relations, which might appropriately be called genealogical, between the symmetries of two point groups (see § 4).

Finally, the study of this theory might be found useful as a preliminary to the heavier work required in the reduction of space groups. In fact, the present work and the examples given here can be considered as a model of the work required in the reduction of the space groups without screws or glides, with the advantage that, owing to the small order of the groups concerned, all the features of the work can be more easily analyzed.

We shall start by revising, in §§ 2 and 3, some well-known properties of the point groups and semi-direct products.

2. Revision on point groups

We shall first consider some concepts that are important in the theory of the proper rotation groups (see Zassenhauss 1949 or, for a fuller treatment, Burckhardt 1947). A basic idea in this theory is that of the *poles* of a rotation, which are the two points of the unit sphere that are left invariant by the rotation: if G_α is a rotation with pole α we can write $G_\alpha \alpha = \alpha$. In general, an operation X will transform the pole α of G_α into another pole β: $X\alpha = \beta$. We say that α and β are *conjugate* and we shall prove that β is the pole of the rotation $XG_\alpha X^{-1}$. In fact

$$XG_\alpha X^{-1}\beta = XG_\alpha X^{-1}X\alpha = XG_\alpha \alpha = X\alpha = \beta. \tag{1}$$

In order to express briefly this result, we define a concept which will be much used in this paper, namely, that of the *conjugation operator*: we note that $XG_\alpha X^{-1}$ can be taken to define an operator $\hat{X}$ that transforms a rotation G_α into another $XG_\alpha X^{-1}$. The relation $\hat{X}G_\alpha \equiv XG_\alpha X^{-1}$ is the definition of the conjugation operator $\hat{X}$. The result that we obtained in (1) can now be stated as follows: if α is the pole of G_α, $X\alpha$ is the pole of $\hat{X}G_\alpha$: $\hat{X}G_\alpha = G_{X\alpha}$.

Until now, we have not made use of group properties. If G_α belongs to a group **G** and $X \in \mathbf{G}$, we say that α and $\beta = X\alpha$ are conjugate under the group **G** and we can see that conjugate poles correspond to conjugate operations, that is, to operations in the same class.

The above considerations are very useful in discussing invariance properties. Let us consider a group of operations **N** with poles $\alpha, \beta, \ldots, \rho$, and assume that **N** is invariant under conjugation with a given operation C, that is, that $\hat{C}N \in \mathbf{N}$ for all $N \in \mathbf{N}$. We can write this more compactly as $\hat{C}\mathbf{N} = \mathbf{N}$. Now the poles of $\hat{C}\mathbf{N}$ are $C\alpha, C\beta, \ldots, C\rho$ and as $\hat{C}\mathbf{N}$ coincides with **N** this set must be the same as $\alpha, \beta, \ldots, \rho$ except perhaps for the order. We conclude that *if* **N** *is invariant under* C, *the latter permutes the poles of* **N**.

Clearly, if **N** is an invariant subgroup of **G** it is invariant under conjugation with every operation of **G**. That is: *the poles of an invariant subgroup are permuted among themselves by all the operations of the group.* As an example, consider the group of the rotations of the cube, **O**. There are three binary axes C_2 parallel to the edges of the cube. Clearly they (and hence their poles) are permuted around by all the operations of the cube. Hence the subgroup made up of the identity and these $3C_2$ (which is the dihedral group $\mathbf{D}_2$) is an invariant subgroup of **O** (as well as of **T** and $\mathbf{T}_d$ as can easily be seen).

Another well-known fact about the poles of a point group is that they separate out into disjointed systems of conjugate poles and this leads to the existence of only ten crystallographic pure rotation groups.

To form the improper rotation groups (that is groups that contain operations other than proper rotations—which can always be given as rotary inversions) we must proceed in either of the two following ways (see Weyl 1952 for a simple proof of this result).

(i) We take any pure rotation group **G** and form the group $\mathbf{G}' = \mathbf{G}+\mathbf{G}i$. Here i is the inversion and the plus sign, as often in this paper, must be understood in the Galois sense as denoting a juxtaposition of elements. Because i commutes with any rotation, the right-hand side here can be written as a direct product $\mathbf{G}' = \mathbf{G}\times\mathbf{C}_i$, where $\mathbf{C}_i = E+i$ and E is the identity element.

(ii) We find a subgroup of **G** of index 2 (hence invariant) which we shall call the *halving subgroup* **H**, and form the improper group $\mathbf{G}' = \mathbf{H}+(\mathbf{G}-\mathbf{H})\,i$ (here $\mathbf{G}-\mathbf{H}$ means the set of elements of **G** that does not belong to **H**). It is easy to find the halving subgroups for all the pure rotation groups, by using the criterion given in the last italicized statement above. For the cyclic groups $\mathbf{C}_n$, $\mathbf{H} = \mathbf{C}_{\frac{1}{2}n}$ (if n is even). For the $\mathbf{D}_n$, $\mathbf{H} = \mathbf{C}_n$ and, if n is even, also $\mathbf{H} = \mathbf{D}_{\frac{1}{2}n}$ (except when $n = 2$ when **H** is the trivial identity group). The only invariant subgroup of **T** is $\mathbf{D}_2$, which is not halving, and for **O** and $\mathbf{T}_d$, $\mathbf{H} = \mathbf{T}$. For future reference, it is important to notice that except for the $\mathbf{C}_n$ the group **G** always possesses poles outside the halving subgroup **H**.

We list in table 1 the ten pure rotation groups and their halving subgroups. It should be noticed that the improper groups obtained as in (i) above contain the inversion as a symmetry operation whereas those from (ii) do not (quite clearly, because $\mathbf{G}-\mathbf{H}$ does not include E). They are listed in the third and fourth columns of the table, respectively.

We wish to express the results given in table 1 in terms of semi-direct products. This we shall do in §4. First, we shall consider in the next section the concept of semi-direct product.

Table 1. Proper and improper rotation groups

proper groups	halving subgroups	groups with i	groups without i
$\mathbf{C}_1$	—	$\mathbf{C}_i$	—
$\mathbf{C}_2$	$\mathbf{C}_1$	$\mathbf{C}_{2h}$	$\mathbf{C}_s$
$\mathbf{C}_3$	—	$\mathbf{C}_{3i}$	—
$\mathbf{C}_4$	$\mathbf{C}_2$	$\mathbf{C}_{4h}$	$\mathbf{S}_4$
$\mathbf{C}_6$	$\mathbf{C}_3$	$\mathbf{C}_{6h}$	$\mathbf{C}_{3h}$
$\mathbf{D}_2$	$\mathbf{C}_2$	$\mathbf{D}_{2h}$	$\mathbf{C}_{2v}$
$\mathbf{D}_3$	$\mathbf{C}_3$	$\mathbf{D}_{3d}$	$\mathbf{C}_{3v}$
$\mathbf{D}_4$	$\mathbf{C}_4$	$\mathbf{D}_{4h}$	$\mathbf{C}_{4v}$
	$\mathbf{D}_2$	—	$\mathbf{D}_{2d}$
$\mathbf{D}_6$	$\mathbf{C}_6$	$\mathbf{D}_{6h}$	$\mathbf{C}_{6v}$
	$\mathbf{D}_3$	—	$\mathbf{D}_{3h}$
$\mathbf{T}$	—	$\mathbf{T}_h$	—
$\mathbf{O}$	$\mathbf{T}$	$\mathbf{O}_h$	$\mathbf{T}_d$

3. Semi-direct products

We do not propose to discuss the most general definition of the semi-direct product: this can be found in the references given in the Introduction, for instance Lomont (1959) Instead, we shall provide a definition adequate for our purposes and which is very simple.†

Consider two groups **N** and **C** which have no common element except the identity and such that **N** is invariant under conjugation with any element of **C**: $\hat{C}\mathbf{N} = \mathbf{N}$, for all $C \in \mathbf{C}$.

† Our definition coincides with that of the 'group product' given by Buerger (1956, p. 486).

Then the set of all the products of one element of **N** times one element of **C** is a group **G**, of which **N** is an invariant subgroup. We call **G** the semi-direct product of **N** and **C**, $\mathbf{G} = \mathbf{N} \wedge \mathbf{C}$. (Notice that this symbol is not commutative: we agree to place the invariant subgroup always first.)

We shall now discuss this definition and prove the theorem given. First, it is important to notice that $\hat{C}\mathbf{N} = \mathbf{N}$ does *not* mean that, for all $N \in \mathbf{N}$, $\hat{C}N = N$, but that $\hat{C}N_i = N_j$ with $N_i, N_j \in \mathbf{N}$. That is, $CN_iC^{-1} = N_j$ or

$$CN_i = N_j C. \tag{2}$$

If we had $N_i = N_j$, (2) would be a commutation relation and the product of **N** times **C** would be a direct product. It is useful to regard (2) as a *quasi-commutation* relation that allows us to alter the order of a product CN_i, as long as we replace N_i by $N_j = \hat{C}N_i$:

$$CN_i = \hat{C}N_i C. \tag{3}$$

Analogously,

$$N_i C = C\hat{C}^{-1}N_i. \tag{4}$$

In these and other relations that contain the operator $\hat{C}$, the reader must carefully understand that $\hat{C}$ must never be separated from the operation on which it acts, that is, that $\hat{C}N$ must be used as a single symbol. For instance, $\hat{C}N_i N_j \neq \hat{C}(N_i N_j)$.

We shall make much use in this paper of the quasi-commutation relations (3) and (4).

In order to prove the theorem, we verify first the existence of the product

$$N_i C_j \,.\, N_k C_l = N_i(\hat{C}_j N_k)\, C_j C_l.$$

Now, because of the condition $\hat{C}\mathbf{N} = \mathbf{N}$, $\hat{C}_j N_k \in \mathbf{N}$ and the right-hand side is a product of an operation of **N** times an operation of **C**, and therefore belongs to the set in question. The remaining group properties are simple to prove and we leave them to the reader.

As an example, consider $\mathbf{N} = \mathbf{C}_3$ and $\mathbf{C} = E + C_2 = \mathbf{C}_2$, where the C_2 axis of the second group is perpendicular to the C_3 axis of the first. (Note that, in giving a semi-direct product of two point groups, it is essential to define unambiguously the setting of the operations of one group with respect to those of the other.) Clearly $\hat{E}\mathbf{C}_3 = \mathbf{C}_3$. Also $\hat{C}_2\mathbf{C}_3 = \mathbf{C}_3$, because C_2 interchanges the two poles (those of the C_3 axis) of $\mathbf{C}_3$ (cf. the first italicized statement in § 2). We can therefore form the group $\mathbf{C}_3 \wedge \mathbf{C}_2$, which is in fact $\mathbf{D}_3$.

Let us consider the *triple semi-direct products*. If $\mathbf{G} = \mathbf{N} \wedge \mathbf{C}$ and $\mathbf{N} = \mathbf{N}' \wedge \mathbf{C}'$, we have $\mathbf{G} = (\mathbf{N}' \wedge \mathbf{C}') \wedge \mathbf{C}$. It can readily be seen that a necessary and sufficient condition for the relation

$$\mathbf{G} = (\mathbf{N}' \wedge \mathbf{C}') \wedge \mathbf{C} = \mathbf{N}' \wedge (\mathbf{C}' \wedge \mathbf{C}) \tag{5}$$

to be valid is that $\mathbf{C}'$ be invariant under **C**. For this to be the case the poles of $\mathbf{N}'$ and $\mathbf{C}'$ must either be all in common or such that no pole of one group is taken into a pole of the other under conjugation with **C**.

4. Point groups as semi-direct products

We shall first prove the following theorem: given a crystallographic point group **G** and a maximal invariant subgroup of it, **N** (that is, an invariant subgroup which is not a subgroup of another invariant subgroup of larger order), the coset representatives of the factor group **G**/**N** are all powers of the same operation of **G**. This is the same as to say that all the coset representatives belong to the same pole of $\mathbf{G}$ (because G and G^2, say, clearly belong to the same pole).

We shall use in the proof the fact that all crystallographic point groups are solvable, that is that they admit of a *composition series*

$$\mathbf{G} \equiv \mathbf{G}_1, \mathbf{G}_2, \mathbf{G}_3, \ldots, \mathbf{G}_m \equiv E,$$

where $\mathbf{G}_{i+1}$ is a maximal invariant subgroup of $\mathbf{G}_i$ and $\mathbf{G}_i/\mathbf{G}_{i+1}$ is cyclic. Let us write for convenience $\mathbf{G}_2 = \mathbf{N}$: the above result means therefore that the factor group

$$\mathbf{G}/\mathbf{N} = \mathbf{N}C_1 + \mathbf{N}C_2 + \ldots + \mathbf{N}C_r \tag{6}$$

is cyclic. Here $r = h/n$ where h and n are the orders of $\mathbf{G}$ and $\mathbf{N}$, respectively, and the C's are the coset representatives. Because $\mathbf{G}/\mathbf{N}$ is cyclic, we can express it in terms of powers of one of the cosets in the right-hand side of (6), which we call $\mathbf{N}C$

$$\mathbf{G}/\mathbf{N} = \mathbf{N}C + (\mathbf{N}C)^2 + \ldots + (\mathbf{N}C)^r. \tag{7}$$

Here $(\mathbf{N}C)^r$ must be equal to the identity element which, as well known for the factor group, is $\mathbf{N}$. That is, $(\mathbf{N}C)^r \equiv \mathbf{N}$. Here, and in (7), we can use the fact that $\mathbf{N}^p = \mathbf{N}$ for all p, and then we obtain

$$\mathbf{G}/\mathbf{N} = \mathbf{N}C + \mathbf{N}C^2 + \ldots + \mathbf{N}C^r, \quad \mathbf{N}C^r \equiv \mathbf{N}, \tag{8}$$

which proves the theorem.

The coset representatives may or may not form a cyclic subgroup of $\mathbf{G}$. In fact, in order to satisfy the condition that appears in (8), one of the two following relations must hold

$$C^r = E, \tag{9}$$

$$C^r \in \mathbf{N}. \tag{10}$$

When (9) is verified, $C + C^2 + \ldots + C^r$ is a group and clearly $\mathbf{G} = \mathbf{N} \wedge \mathbf{C}$. If it is not possible to find a suitable coset representative $C \in \mathbf{G}$ for which (9) obtains, it means that for all such C's (10) is valid, that is, that there is no pole in $\mathbf{G}$ outside those of $\mathbf{N}$. As this can be the case only for cyclic groups (see the remark at the end of of § 2), we have shown that all proper rotation groups, except perhaps some cyclic groups, can be written as semi-direct products, the second factor of which is always a cyclic group. This means of course that we are able to express the proper rotation groups as semi-direct products in all cases of practical interest: the cyclic groups are so easy to handle that it is not of much use to be able to factorize them. However, even these (written $\mathbf{C}_n$) will factorize when their order n is an even number such that $\frac{1}{2}n$ is odd: $\mathbf{N} = \mathbf{C}_{\frac{1}{2}n}$ and $C = C_2$ so that $C_2^2 = E$ and (9) is satisfied.

It is now very easy to form semi-direct products for all the point groups, by inspecting table 1. As an example, $\mathbf{D}_3 = \mathbf{C}_3 + \mathbf{C}_3 C_2 = \mathbf{C}_3 \wedge (E + C_2) = \mathbf{C}_3 \wedge \mathbf{C}_2$. To form the corresponding improper group under the rule (ii) of § 2, it is necessary to multiply by i all the operations in $\mathbf{D}_3$ that do not belong to $\mathbf{C}_3$; the group is: $\mathbf{C}_3 \wedge (E + iC_2) = \mathbf{C}_3 \wedge \mathbf{C}_s \equiv \mathbf{C}_{3v}$. (It can easily be seen that, in fact, i does not affect the invariance.) In general, if we consider the proper point groups of the first column of table 1 they are (except $\mathbf{C}_4$, see above) given by the semi-direct product of the halving (invariant) subgroup in the second column times a group $\mathbf{C}_2$, whereas the semi-direct product of the same invariant subgroup times a group $\mathbf{C}_s$ will yield all the improper groups without inversion which are given in the last column of table 1. $\mathbf{T}$ does not possess a halving subgroup, but as already shown before (§2) $\mathbf{D}_2$ is an invariant subgroup of it which generates a semi-direct product expression for $\mathbf{T}$. The improper groups with the inversion are not considered, because they are more simply given as direct products (however, see below). We summarize these results in table 2. In using semi-direct products attention must be paid (see the $\mathbf{C}_{3v}$ example in §3) to the relative orientation of the axes of the two factors and in order to do this we use a rotation explained in the note at the head of the table.

Table 2. The point groups as semi-direct products

$\mathbf{C}_2$ and $\mathbf{C}_s$ are groups with the rotation axis and mirror plane parallel and perpendicular, respectively, to the principal axis of the invariant subgroup. The rotation axis and mirror plane in $\mathbf{C}_2'$ and $\mathbf{C}_s'$ are perpendicular and parallel, respectively, to the principal axis. The symmetry elements in $\mathbf{C}_2''$ and $\mathbf{C}_s''$ are as in $\mathbf{C}_2'$ and $\mathbf{C}_s'$ but they also bisect two secondary axes of the invariant subgroup. The C_3 axis of $\mathbf{C}_3'$ and $\mathbf{D}_3'$ is diagonal to the three C_2 axes of $\mathbf{D}_2$.

proper rotation groups		improper rotation groups (without i)	
name of group	semi-direct product form	semi-direct product form	name of group
$\mathbf{C}_1$	—	—	—
$\mathbf{C}_2$	$\mathbf{C}_1 \wedge \mathbf{C}_2$	$\mathbf{C}_1 \wedge \mathbf{C}_s$	$\mathbf{C}_s$
$\mathbf{C}_3$	—	—	—
$\mathbf{C}_4$	—	—	$\mathbf{S}_4$
$\mathbf{C}_6$	$\mathbf{C}_3 \wedge \mathbf{C}_2$	$\mathbf{C}_3 \wedge \mathbf{C}_s \equiv \mathbf{C}_3 \times \mathbf{C}_s$	$\mathbf{C}_{3h}$
$\mathbf{D}_2$	$\mathbf{C}_2 \wedge \mathbf{C}_2' \equiv \mathbf{C}_2 \times \mathbf{C}_2'$	$\mathbf{C}_2 \wedge \mathbf{C}_s' \equiv \mathbf{C}_2 \times \mathbf{C}_s'$	$\mathbf{C}_{2v}$
$\mathbf{D}_3$	$\mathbf{C}_3 \wedge \mathbf{C}_2'$	$\mathbf{C}_3 \wedge \mathbf{C}_s'$	$\mathbf{C}_{3v}$
$\mathbf{D}_4$	$\mathbf{C}_4 \wedge \mathbf{C}_2'$	$\mathbf{C}_4 \wedge \mathbf{C}_s'$	$\mathbf{C}_{4v}$
	$\mathbf{D}_2 \wedge \mathbf{C}_2''$	$\mathbf{D}_2 \wedge \mathbf{C}_s'' = \mathbf{S}_4 \wedge \mathbf{C}_2'$	$\mathbf{D}_{2d}$
$\mathbf{D}_6$	$\mathbf{C}_6 \wedge \mathbf{C}_2'$	$\mathbf{C}_6 \wedge \mathbf{C}_s'$	$\mathbf{C}_{6v}$
	$\mathbf{D}_3 \wedge \mathbf{C}_2''$	$\mathbf{D}_3 \wedge \mathbf{C}_s'' = \mathbf{S}_3 \wedge \mathbf{C}_2'$	$\mathbf{D}_{3h}$
$\mathbf{T}$	$\mathbf{D}_2 \wedge \mathbf{C}_3'$	—	—
$\mathbf{O}$	$\mathbf{T} \wedge \mathbf{C}_2'' = \mathbf{D}_2 \wedge \mathbf{D}_3'$	$\mathbf{T} \wedge \mathbf{C}_s'' = \mathbf{D}_2 \times \mathbf{C}_{3v}$	$\mathbf{T}_d$

A few comments about the expressions in table 2: first, it should be noticed that the improper groups with inversion derived from $\mathbf{D}_n$ (n even) admit a cyclic group $\mathbf{S}_m$ as an invariant subgroup, and that therefore an alternative form for their semi-direct product expression can be written, which might be sometimes advantageous because both factors are cyclic. Secondly, the factorization in semi-direct products can be iterated as shown at the end of §3 (see equation (5)). In particular we saw that if $\mathbf{A}$ and $\mathbf{B}$ have all or no poles in common the triple product can be written as $(\mathbf{A} \wedge \mathbf{B}) \wedge \mathbf{C} = \mathbf{A} \wedge (\mathbf{B} \wedge \mathbf{C})$ which provides a new form for the product $\mathbf{N} \wedge \mathbf{C}$ if $\mathbf{N} = \mathbf{A} \wedge \mathbf{B}$. Since we have always chosen $\mathbf{C}$ so that the required conditions are satisfied, this decomposition is always possible and sometimes convenient, because it gives an alternative semi-direct product with an invariant subgroup of lower order. This is particularly useful when $\mathbf{N}$ is not Abelian, because it allows us to reduce it until it becomes so. As an example, from the table,

$$\mathbf{O} = (\mathbf{D}_2 \wedge \mathbf{C}_3') \wedge \mathbf{C}_2'' = \mathbf{D}_2 \wedge (\mathbf{C}_3' \wedge \mathbf{C}_2'') = \mathbf{D}_2 \wedge \mathbf{D}_3'.$$

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This shows that all point groups can be expressed in terms of semi-direct products the invariant subgroups of which are cyclic. This result complements the theorem given at the beginning of this section.

As we have said, the improper groups with inversion are most simply expressed by direct products of the ten proper point groups with $\mathbf{C}_i$, say $\mathbf{M} \times \mathbf{C}_i$. Nevertheless, they can always be expressed as semi-direct products. It can readily be seen that this is so because the *mixed triple product* $(\mathbf{A} \wedge \mathbf{B}) \times \mathbf{C}$ satisfies the relation

$$(\mathbf{A} \wedge \mathbf{B}) \times \mathbf{C} = \mathbf{A} \wedge (\mathbf{B} \times \mathbf{C}). \tag{11}$$

Of course, the proper point groups $\mathbf{M}$ can always be written $\mathbf{M} = \mathbf{A} \wedge \mathbf{B}$ from table 2 and therefore (11) will yield the required expression. For instance,

$$\mathbf{D}_{4h} = \mathbf{D}_4 \times \mathbf{C}_i = (\mathbf{C}_4 \wedge \mathbf{C}_2') \times \mathbf{C}_i = \mathbf{C}_4 \wedge \mathbf{C}_{2h}.$$

Many new expressions can be written by exploiting the properties discussed for the triple and mixed triple products. We leave them to the reader with a warning that, if they are used, care should be exercised in specifying the relative setting of the groups that finally appear in the products. It should be noticed that relations of this type are interesting not only for academical reasons: they provide a very good method for establishing genealogical relations between two groups, as appear, for instance, when the symmetry of a system is increased or reduced by some perturbation.

Much of the importance of the semi-direct product arises from the fact that its irreducible representations can be built up from those of its factors, as we shall see in the next section.

5. The representations of the semi-direct product

We shall follow closely in this section a method used by Johnston (1960) to discuss the reduction of space groups. We first review two general theorems, proofs of which can be found in that paper.

(a) *Reducibility condition for a group expressed in terms of the cosets of one of its subgroups*

Let us consider a group $\mathbf{G}$ with a subgroup $\mathbf{H}$. $\mathbf{G}$ can be written as a sum of cosets of $\mathbf{H}$: $\mathbf{G} = \sum_i \mathbf{H} C_i$ where the summation sign must be understood in the Galois sense (i.e. as a juxtaposition) and the C_i's are the coset representatives of $\mathbf{H}$. We shall agree to take always $C_1 = E$. Also we shall write the basis of our representations as *row* vectors denoted with a symbol such as $\langle\phi|$ (ϕ here represents one typical partner of the several functions of the basis). Consider now $\langle\phi|$, an irreducible basis under $\mathbf{H}$. It can then be proved that $\Lambda = \sum_i C_i \langle\phi|$ (symbolic summation again: direct sum) is an invariant space, and hence a basis, of the whole group $\mathbf{G}$. The first question is whether this basis is irreducible. This is answered as follows:

Split Λ in subspaces $\Lambda_i = C_i\langle\phi|$: it can be proved that Λ_i is invariant under the group $\hat{C}_i \mathbf{H} \equiv \mathbf{H}_i$†. Consider now any two such spaces, Λ_i and Λ_j. They span representations of

† An example of the invariance of Λ and Λ_i can be found in § 5 (*b*).

$\mathbf{H}_i$ and $\mathbf{H}_j$ of characters χ^i and χ^j, respectively. If $\mathbf{H}_{ij}$ denotes the set of all operations R common to $\mathbf{H}_i$ and $\mathbf{H}_j$, the irreducibility condition of Λ under $\mathbf{G}$ is

$$\sum_{R\in\mathbf{H}_{ij}} \chi^i(R)^* \chi^j(R) = 0, \quad \text{wherever} \quad i \neq j, \tag{12}$$

but this is valid only if the spaces Λ_i and Λ_j are orthogonal for all i and j.

The second question is this: if Λ, generated in the way shown above by the basis $\langle\phi|$ that belongs to the ith irreducible representation of $\mathbf{H}$ of characters $\chi^i(H)$, is reducible under $\mathbf{G}$, how many times will the jth irreducible representation of $\mathbf{G}$ appear in the reducible one spanned by Λ? In order to answer this, notice that the matrices of the jth representation of $\mathbf{G}$ that correspond to $\mathbf{H}$ form a representation of $\mathbf{H}$: find the number of times that it contains the ith representation. This is the same as the number of times that the jth representation of $\mathbf{G}$ is contained in Λ.

(*b*) *The star of the representation*

Much of this section will be devoted to a proof of the invariance of the spaces Λ and Λ_i discussed in § 5 (*a*), now for the particular case of the semi-direct product. We do this in order to introduce some concepts which are very useful in dealing with such groups.

Consider $\mathbf{G} = \mathbf{N} \wedge \mathbf{C}$ where the orders of $\mathbf{N}$ and $\mathbf{C}$ are $h_{\mathbf{N}}$ and $h_{\mathbf{C}}$, respectively, and identify $\mathbf{N}$ with the subgroup $\mathbf{H}$ of § 5 (*a*). Take a basis $\langle\phi|$ of n functions that spans the kth irreducible n-dimensional representations of $\mathbf{N}$:

$$N_u\phi_r = \sum_s \phi_s D^k(N_u)_{sr} \quad (u = 1, 2, \ldots, h_{\mathbf{N}}). \tag{13}$$

Here the coefficients $\mathrm{D}^k(N_u)_{sr}$ are the sr matrix elements of the matrix representative of N_u in this representation. We now form the functions

$$\phi_{vr} = C_v\phi_r \quad (v = 1, \ldots, h_{\mathbf{C}};\ r = 1, \ldots, n) \tag{14}$$

(since we always take $C_1 = E$, $\phi_{1r} \equiv \phi_r$) and we shall prove that they form a space Λ which is invariant under $\mathbf{G}$. Consider a typical element of $\mathbf{G}$, $G_{pq} \equiv N_p C_q$,

$$N_p C_q \phi_{vr} = N_p C_q C_v \phi_r. \tag{15}$$

We write $C_q C_v = C_\tau \in \mathbf{C}$ and we use the quasi-commutation relation (4) on the product $N_p C_\tau$ that now appears on the right-hand side of (15)

$$N_p C_q \phi_{vr} = C_\tau \hat{C}_\tau^{-1} N_p \phi_r. \tag{16}$$

Since $\hat{C}_\tau^{-1} N_p \in \mathbf{N}$ we can introduce (13) into this equation

$$N_p C_q \phi_{vr} = C_\tau \sum_s \phi_s D^k(\hat{C}_\tau^{-1} N_p)_{sr} = \sum_s \phi_{\tau s} D^k(\hat{C}_\tau^{-1} N_p)_{sr}. \tag{17}$$

Equation (17) gives the transform of any function ϕ_{vr} of Λ under an operation of $\mathbf{G}$ in terms of functions of the same space Λ, which proves the invariances of the latter.

Consider now the subspaces Λ_i, spanned by the functions

$$\phi_{ir} = C_i \phi_r \quad (r = 1, 2, \ldots, n). \tag{18}$$

We shall prove that Λ_i spans a representation of $\mathbf{N}$:

$$\begin{aligned} N_p \phi_{ir} = N_p C_i \phi_r &= C_i \hat{C}_i^{-1} N_p \phi_r \\ &= C_i \sum_s \phi_s D^k(\hat{C}_i^{-1} N_p)_{sr} \\ &= \sum_s \phi_{is} D^k(\hat{C}_i^{-1} N_p)_{sr}. \end{aligned} \tag{19}$$

The representation $D^k(\hat{C}_i^{-1}N)$ is one derived from the original representation $D^k(N)$ of (13) by establishing the automorphism $N \to \hat{C}_i^{-1}N$ (remember that $\hat{C}_i^{-1}N$ must belong to **N** because the latter is invariant under **G**). Two representations connected in this way are called *conjugate* (see, for instance, Lomont 1959, p. 221) and in order to be able to express briefly the relation between two conjugate representations we call $\hat{\mathscr{C}}_i D^k$ the representation conjugate to D^k under $\hat{C}_i$, that is we define an operator $\hat{\mathscr{C}}_i$ such that

$$\hat{\mathscr{C}}_i D^k(N) = D^k(\hat{C}_i^{-1}N). \tag{20}$$

It must be clearly understood that two conjugate representations are not in general equivalent: if $C_i \notin \mathbf{N}$, $\hat{C}_i^{-1}N$ and N do not belong in general to the same class of **N** and therefore the two conjugate representations do not have the same characters.† On the other hand, although the same element will have a different character in $D^k(N)$ and in $\hat{\mathscr{C}}_i D^k(N)$, the characters that appear in both representations must be the same except for the order. Hence, as we have chosen D^k to be irreducible, $\hat{\mathscr{C}}_i D^k$, which is the representation spanned by Λ_i, will also be irreducible.

It is now clear that the space Λ contains all the irreducible representations of **N** derived from the original one D^k by acting upon it with all the operators $\hat{\mathscr{C}}_i$ corresponding to **C**. It can also be proved (see Koster 1957, p. 216, for a proof of a similar case that can easily be adapted here) that there are no other representations in Λ. Summarizing, Λ contains all the representations $\hat{\mathscr{C}}_i D^k$ (all $\hat{\mathscr{C}}_i$ in **C**) and only these. A set of representations thus derived from a given irreducible representation of the invariant subspace **N** of $\mathbf{G} = \mathbf{N} \wedge \mathbf{C}$ is called the *star* of the representation of **G**: every representation of **G** must contain only such representations of **N** as appear in one star.‡

We now wish to find out whether a star, that is the space Λ, is irreducible under the group **G**. We shall discuss in this section the particular case when the star does not contain any two representations of **N** that are equivalent. Hence, the spaces Λ_i and Λ_j, which span inequivalent representations $\hat{\mathscr{C}}_i D^k$ and $\hat{\mathscr{C}}_j D^k$, respectively, are orthogonal and we can apply the criterion given by (12) of § 5 (*a*). We know that Λ_i and Λ_j span representations of **N** (which of course also follows from the results quoted in § 5 (*a*): $\mathbf{H}_i = \hat{C}_i^{-1}\mathbf{N} = \mathbf{N}$, $\mathbf{H}_j = \hat{C}_j^{-1}\mathbf{N} = \mathbf{N}$). Hence $\mathbf{H}_{ij} \equiv \mathbf{N}$ and condition (12) reads

$$\sum_{\mathbf{N}} \chi^i(N)^* \chi^j(N) = 0, \quad \text{for all } i \neq j, \tag{21}$$

which is the case because the representations spanned by Λ_i and Λ_j are supposed to be inequivalent.

An example of an irreducible representation of **G** for which the condition assumed in this section is valid will be given in § 6 for the representation E of the group $\mathbf{C}_{3v}$. In this

† The reader must not try to prove that $D^k(\hat{C}_i^{-1}N)$ and $D^k(N)$ are equivalent by writing

$$D^k(\hat{C}_i^{-1}N) = D^k(C_i^{-1}NC_i) = D^k(C_i^{-1})\, D^k(N)\, D^k(C_i).$$

This is fallacious because the basis $\langle\phi|$ that spans a representation on **N** does not in general span a representation of **C**: the symbol $\mathbf{D}^k(C_i)$ is meaningless and the symbol $D^k(\hat{C}_i^{-1}N)$ must be understood as explained in the text.

‡ It is usual in the literature on the semi-direct product (see Lomont 1959) to designate what we have called a star with the name *orbit*, introduced by Mackey. We follow McIntosh (1958) in keeping a terminology which parallels that due to Bouckaert *et al.* (1936), which is standard in the theory of space groups.

and in similar cases one starts with a basis $\langle\phi|$ (representation D^k), generates all the bases $C_i\langle\phi|$ and finds that the $\hat{\mathscr{C}}_i D^k$ (all $C_i \in \mathbf{C}$) are inequivalent to D^k. The space obtained spans, in accordance with the treatment of this section, an irreducible representation of **G**, most simply generated as we have seen from one representation of **N**. Unfortunately, not all the irreducible representations of a group **G** can be obtained in this way, that is to say, there are stars that possess equivalent representations. The question of their irreducibility will be answered in the next section.

(*c*) *The little group*

Suppose now that some of the representations $\hat{\mathscr{C}}_i D^k(N)$ (for all $\hat{\mathscr{C}}_i$ in **C**) are equivalent to the representation $D^k(N)$ that generates the star. It can readily be seen that the set of all operations C_i of **C** for which $\hat{\mathscr{C}}_i D^k(N)$ is equivalent to $D^k(N)$ forms a group which we shall call $\bar{\mathbf{K}}$. In order to prove the irreducibility of the representations, it is more convenient to work with a supergroup of $\bar{\mathbf{K}}$ that includes *all* the operations of **G** for which $\hat{\mathscr{G}} D^k(N)$ is equivalent to $D^k(N)$. This is called the *little group* **K** or, to adopt a terminology similar to the one current in the work on space groups, *the group of k*.† It is clear that **K** contains **N** and $\bar{\mathbf{K}}$ as subgroups, and that it can be written $\mathbf{K} = \mathbf{N} \wedge \bar{\mathbf{K}}$. It is important for the purposes of the present section that the reader should carefully distinguish between **K** and $\bar{\mathbf{K}}$. To stress this distinction we shall call the latter the *little co-group* (or the *co-group of k*), since it is made up of the coset representatives of **K** with respect to **N**. For the purposes of the proofs of this section we shall utilize the little group, but in practice, of course, it is desirable to use the little co-group; how the passage from one to the other is made, when possible, will be shown at the end of this section.

In order to consider stars that contain equivalent representations we express **G** afresh, now in terms of its cosets with respect to **K** rather than those with respect to **N** as in the last section. That is, we write $\mathbf{G} = \sum_i \mathbf{K} S_i$, where, if we refer to § 5 (*a*) the symbols **K** and S_i take the place of **H** and C_i, respectively. We can now form the representation spaces described in § 5 (*a*), and accept their invariance properties as enunciated in that section. We can choose the basis $\langle\phi|$ irreducible under **K** (see § 5 (*a*)) so that at least one of the functions of $\langle\phi|$ belongs to the star of D^k under consideration, say to the representation D^k itself that generates the star. It is now simple to prove that all the functions of $\langle\phi|$ must belong to D^k and correspondingly that all the functions of $\Lambda_i = S_i\langle\phi|$ belong to $\hat{\mathscr{S}}_i D^k$.‡ $\hat{\mathscr{S}}_i D^k$ and $\hat{\mathscr{S}}_j D^k$ can never be equivalent, because S_i and S_j belong to **K**. Hence the two corresponding spaces Λ_i and Λ_j must be orthogonal and we can apply the irreducibility condition (12) of § 5 (*a*). In order to do this we first note that the corresponding subgroups under which Λ_i and Λ_j are invariant, $\mathbf{K}_i = \hat{S}_i \mathbf{K}$ and $\mathbf{K}_j = \hat{S}_j \mathbf{K}$, respectively, admit **N** as a subgroup. Hence $\mathbf{K}_{ij}$, the group of elements common to $\mathbf{K}_i$ and $\mathbf{K}_j$, admits **N** as a subgroup, so that when considering the sum $\sum_{R\in\mathbf{K}_{ij}} \chi^i(R)^* \chi^j(R)$ we can use the reducibility condition described in

† It should be remembered that k is the index that denotes an irreducible representation of the invariant subgroup. For the space groups, these irreducible representations are identified by the so-called **k** vector and the little group is the *group of the* **k** *vector*.

‡ In order to do this write $\mathbf{K} = \mathbf{N} \wedge \bar{\mathbf{K}}$ and apply the theory of the last section, with **K** in the place of **G** and $\bar{\mathbf{K}}$ in that of **C**. Since $\langle\phi|$ spans a representation of **K** it can contain functions of one star only. The star is now generated by the operations of $\bar{\mathbf{K}}$. As these are such as to leave D^k invariant, no other representation except D^k can be found in the star and hence in the representation spanned by $\langle\phi|$.

the last paragraph of § 5 (*a*). In accordance with this, the reducible representation $\chi^i(R)$ (all $R \in \mathbf{K}_{ij}$) contains an irreducible one $\chi^m(R)$ just as many times as the representation of **N** given by $\chi^m(R)$ (all $R \in \mathbf{N}$) contains a certain irreducible representation of **N**, $\chi^\mu(R)$. We know that if $\chi^\mu(R)$ $(R \in \mathbf{N})$ appears in $\chi^j(R)$ $(R \in \mathbf{K}_{ij})$ it cannot appear in $\chi^i(R)$ (because $\mathbf{K}_i$ and $\mathbf{K}_j$ have no representation of **N** in common). Hence the irreducible representation $\chi^m(R)$ $(R \in \mathbf{K}_{ij})$ cannot appear in both $\chi^i(R)$ and $\chi^j(R)$ and the sum in question must vanish, which proves the irreducibility of the representation of **G** that corresponds to the given star.

We have now seen that an irreducible representation of $\mathbf{G} = \mathbf{N} \wedge \mathbf{C}$ is fully determined by the star of the representation, and one irreducible representation of the little group. But the star has now been re-defined: if D^k is the representation used of the group **K** of the star, the latter is obtained by adding to D^k all the representations $\hat{\mathscr{G}}_i D^k$, for all $G_i \in \mathbf{G}$ that do not belong to **K**. From the point of view of forming the bases for the irreducible representations of **G** this result means that we can always form a basis $\langle\phi|$ that spans both an irreducible representation $D^k(N)$ of **N** and an irreducible representation of the little group **K** of D^k: on forming the functions $G_i\langle\phi|$ (all G_i not in **K**) and taking their direct sum we obtain a basis of an irreducible representation of **G**. An example of this situation will appear in § 6 for the group $\mathbf{C}_{3v}$ (see table 3). In accordance with the procedure of the last section the representation A_1 would appear twice in the star. It will be shown in § 6 that for this representation $\mathbf{K} \equiv \mathbf{C}_{3v}$, whence, the group of the operations of **G** not in **K** being void, the re-defined star contains A_1 only.

Although the above results are important, the theory requires further elaboration in order to lead to a practical method for reducing **G**. This is so because in the above process we require the previous reduction of **K** which may indeed coincide with **G** (this is in fact often the case) and then the method suggested by our theorem leaves us almost where we were before using it. It is in order to avoid this difficulty that we must try to replace the use of the little group **K** by that of the little co-group $\bar{\mathbf{K}}$, which must always be of lower order.

We shall first consider the case when the invariant subgroup **N** is Abelian. Consider the space Λ_1 as defined in this section, spanned by a basis $\langle\phi|$ and irreducible under **K**. The matrices $D^k(N)$ on this basis can always be assumed to be diagonal if **N** is Abelian (because as they commute they can all be taken to diagonal form by a similarity transformation). Also, because $\mathbf{K} = \mathbf{N} \wedge \bar{\mathbf{K}}$ the basis $\langle\phi|$ must span matrix representatives for all $C \in \bar{\mathbf{K}}$, and since the $D^k(N)$ are diagonal, if the $D^k(C)$ $(C \in \bar{\mathbf{K}})$ are reduced then clearly the representation of **K** is also reduced, against the assumption. That is, if the representation spanned by $\langle\phi|$ (space Λ_1) is irreducible under **K** it must also be irreducible under $\bar{\mathbf{K}}$. It should also be noticed that the direct sum of the $G_i\langle\phi|$ (all G_i not in **K**) is the same as that of $C_i\langle\phi|$ (all C_i not in $\bar{\mathbf{K}}$). In this manner we work entirely in terms of the group $\bar{\mathbf{K}}$.

Clearly, the above result is also valid in a second case, namely, when **N** is not Abelian but Λ_1 is one-dimensional, that is, when the representations of the star are all one-dimensional. Before we deal with the third and most general case (**N** not Abelian, Λ_1 multi-dimensional), we shall show how, in the two cases already considered, the reduction of $\mathbf{G} = \mathbf{N} \wedge \mathbf{C}$ can be most simply effected. We first find the irreducible (one-dimensional) representations of **N**. We take one of them, $D^k(N)$ and form its star $\hat{\mathscr{C}}D^k(N)$ for all $C \in \mathbf{C}$ and find the operations for which $\hat{\mathscr{C}}D^k(N)$ is equivalent (in fact identical on account of the non-degeneracy of the representation). These operations form the little co-group $\bar{\mathbf{K}}$. (In § 6 a method will be given whereby this part of the work becomes trivial for the point groups.) We now find the irreducible representations of $\bar{\mathbf{K}}$ (which is itself a point group, smaller than $\mathbf{G}$ and which can be assumed to have been previously reduced: very often, $\bar{\mathbf{K}}$ cannot be more involved than $\mathbf{C}_2$, as can be seen from table 2) and take a basis $\langle\phi|$ that spans one of the irreducible representations of $\bar{\mathbf{K}}$ and that belongs to the representation $D^k(N)$ of the star under consideration. (This basis forms the space Λ_1 above.) Finally, we form the functions $C\langle\phi|$ for all $C \in \mathbf{C}$ not in $\bar{\mathbf{K}}$, which form the desired partners of $\langle\phi|$ in the irreducible representation given by the star of D^k. (The latter are the subspaces Λ_2, Λ_3, etc.)

It must be clearly understood that although Λ_1 spans an irreducible representation of $\bar{\mathbf{K}}$, the space $\Lambda = \sum_i \Lambda_i$ (in direct sum sense) which spans the irreducible representation of the star and a *reducible* representation of $\bar{\mathbf{K}}$, contains representations of $\bar{\mathbf{K}}$ other than that spanned by Λ_1. This is so because there is no reason whatever why the basis $C\langle\phi|$ should span the same irreducible representation of $\bar{\mathbf{K}}$ as $\langle\phi|$.†

It is also useful to remark that in both cases treated above, when two representations of the star, say $\hat{\mathscr{C}}_i D^k$ and $\hat{\mathscr{C}}_j D^k$, are equivalent, they must be identical, that is, representations of $\mathbf{N}$ can at most be repeated within a star. If we consider the way in which an irreducible representation of $\mathbf{G} = \mathbf{N} \wedge \mathbf{C}$ is formed, it is clear that this can only happen when the representation used of the little co-group $\bar{\mathbf{K}}$ (sometimes called the *small representation*) is multi-dimensional. Since $\bar{\mathbf{K}}$ is a subgroup of $\mathbf{C}$ and the latter can be taken always to be cyclic in the first instance, this will be only the case when, $\mathbf{N}$ being non-Abelian, $\mathbf{G}$ is expressed as a triple semi-direct product (such as was the case for $\mathbf{O}$ in the example of § 4).

In principle, the two cases considered, or rather the first one by itself, solve for us the question of the reduction of point groups, as we have seen (§ 4) that they can all be written in terms of semi-direct products with an Abelian first factor. Nevertheless, the third and more general case is of practical interest, because, as we have already stressed, the general semi-direct product expressions are very useful in relating the irreducible representations of a group to those of an invariant subgroup, not necessarily Abelian. It is simple to see what will now happen, when $D^k(N)$, the representation used to generate the star, is multi-dimensional: the representation spanned by $\langle\phi|$ (space Λ_1), irreducible under $\mathbf{K}$ is no longer irreducible under $\bar{\mathbf{K}}$. Λ_1 spans now a reducible representation of $\bar{\mathbf{K}}$ and we cannot use the procedure applicable in the previous cases. The complete theory of the method now required becomes rather involved (see Lomont 1959; McIntosh 1958), but for the point groups it is possible to circumvent this difficulty by exploiting the fact that, if $\mathbf{G} = \mathbf{N} \wedge \mathbf{C}$ and $\mathbf{N}$ is not Abelian, the latter can be further factorized until an Abelian subgroup appears as prefactor. We shall assume that in fact $\mathbf{N} = \mathbf{N}' \wedge \mathbf{C}'$ where $\mathbf{N}'$ is Abelian and $\mathbf{C}'$ is cyclic of prime order. For this particular case, which is the only one that arises for the point groups, the theory is very simple.

We shall first give a general result for the semi-direct product $\mathbf{N} = \mathbf{N}' \wedge \mathbf{C}'$, with $\mathbf{N}'$ Abelian and $\mathbf{C}'$ cyclic of prime order: if $D^k(N)$ is multi-dimensional its corresponding little co-group must be $\mathbf{C}_1$ (the identity only). In fact, $D^k(N)$ must correspond to the star of, say, $D^j(N')$ and because $\mathbf{C}'$ is cyclic this star cannot contain repeated representations.

† An example of this situation can be found at the end of § 8 (*c*).

Therefore, at least some operations of $\mathbf{C}'$ must generate representations $\hat{\mathscr{C}}'D^j(N')$ different from $D^j(N')$, that is the little co-group of $D^j(N')$ must be smaller than $\mathbf{C}'$: also it must be a subgroup of $\mathbf{C}'$. As a cyclic group of prime order admits $\mathbf{C}_1$ only as a proper subgroup our result is proved. (It should be noticed that this result also means that each operation of $\mathbf{C}'$ generates a different column of the representation $D^k(N)$.)

Consider a representation of $\mathbf{G} = \mathbf{N} \wedge \mathbf{C} = \mathbf{N}' \wedge \mathbf{C}' \wedge \mathbf{C}$ corresponding to the star generated by the multi-dimensional representation $D^k(N)$, with group $\bar{\mathbf{K}}_{\mathbf{C}}$. (The suffix here identifies the little co-group in an obvious manner.) Because $\mathbf{N} = \mathbf{N}' \wedge \mathbf{C}'$, $D^k(N)$ is, in its turn, generated by the (one-dimensional) representation $D^j(N')$, the little co-group of which, here denoted with $\bar{\mathbf{J}}_{\mathbf{C}'}$, is equal to $\mathbf{C}_1$ in accordance with the result just obtained.

We now write $\mathbf{G} = \mathbf{N}' \wedge \mathbf{C}' \wedge \mathbf{C} = \mathbf{N}' \wedge \mathbf{C}''$, say, and the irreducible representation of $\mathbf{G}$ in question must be generated by $D^j(N')$ with a little co-group $\bar{\mathbf{J}}_{\mathbf{C}''}$. It can be seen that $\bar{\mathbf{J}}_{\mathbf{C}''} = \bar{\mathbf{J}}_{\mathbf{C}'} \wedge \bar{\mathbf{K}}_{\mathbf{C}} = \mathbf{C}_1 \wedge \bar{\mathbf{K}}_{\mathbf{C}} = \bar{\mathbf{K}}_{\mathbf{C}}$. This means, in accordance with our result for Abelian invariant subgroups, that the basis of $D^j(N')$ can be chosen to belong to one of the irreducible representations of $\bar{\mathbf{K}}_{\mathbf{C}}$. But the basis of $D^j(N')$ is clearly a partner in $D^k(N)$, that is, a function that belongs to one of the columns of $D^k(N)$. Hence, we have proved the following result: under the conditions stated, $D^k(N)$ can be chosen so that one of its columns belongs to the little co-group of its star. Of course, the formation of $D^k(N)$ itself is no problem, as it must be provided by the factorization $\mathbf{N} = \mathbf{N}' \wedge \mathbf{C}'$. An application of this result will be found in § 8 (*c*).

(*d*) *The representations*

We have now all the necessary tools to derive the representations for the point groups. Given $\mathbf{G} = \mathbf{N} \wedge \mathbf{C}$ we know that in an irreducible representation $D^j(G)$ the matrices for $D^j(N)$ will be direct sum of matrices $D^k(N)$, $D^{k'}(N)$, etc., that span irreducible representations of $\mathbf{N}$. They are all generated from $D^k(N)$ by forming $\hat{\mathscr{C}}D^k(N)$ for all $C \in \mathbf{C}$. Also, we know how to select $D^k(N)$, the generator of the star: if it is one-dimensional, it must belong to one of the irreducible representations of the co-group of the star and if it is not then, under certain conditions (see § 5 (*c*)), one of its columns must belong to the co-group of the star. These conditions fully determine the matrices $D^j(N)$, as will be clear when we consider some examples (see § 8). Once we know the matrices $D^j(N)$ we must also know, or otherwise we can easily determine by standard methods (see § 7) the bases of the representations. It is enough to transform these bases under all the operations of $\mathbf{C}$ (which as we have seen is most often a very simple group such as $\mathbf{C}_2$) and therefore we have, by multiplication, matrices for the whole group $\mathbf{G}$.

There is a useful result about the general form of the matrices $D^j(C)$ for the particular case when all the representations of the star are one-dimensional and different. This follows from the way in which we generate a basis for the representation by forming the subspaces Λ_1, Λ_2, etc., of § 5 (*c*). Λ_1 will now be just a function ϕ_1, that belongs to one of the representations of $\bar{\mathbf{K}}$, which will be assumed larger than $\mathbf{C}_1$. We shall normally write this function as the first or last of the basis and shall call it the *pivot* of the representation. ϕ_1 belongs to an irreducible representation of $\mathbf{N}$ and the other functions ϕ_2, ϕ_3, etc., of the star (spaces $\Lambda_2, \Lambda_3, \ldots$), generated by $C\phi_1$, with $C \notin \bar{\mathbf{K}}$, belong to different irreducible representations of $\mathbf{N}$. When $C \in \bar{\mathbf{K}}$ it leaves the pivot invariant, but multiplies it, of course, by whatever numerical factor that corresponds to the irreducible representation of $\bar{\mathbf{K}}$ in question. This factor will appear in the diagonal matrix element of $D^j(C)$ that corresponds to the same column as the pivot. When $C \notin \mathbf{K}$ it interchanges the functions $\phi_1, \phi_2, \phi_3, \ldots$ in such a way that the pivot is always taken out of position: $D^j(C)$ will be such that the diagonal matrix element corresponding to the pivot vanishes and the other matrix elements are those of $D^j(N)$ but in general, in different positions.

When $\mathbf{C} = \mathbf{C}_2$, which is often the case, the functions that are not pivotal are just interchanged by C_2, as can be readily demonstrated. Hence the diagonal elements of their matrices must always vanish.

Of course, when $D^k(N)$ is diagonal, if a diagonal matrix element of $D^k(C)$ vanishes, the corresponding matrix element for all $G \in \mathbf{G}$ must also vanish.

It should be noticed that when $\overline{\mathbf{K}} = \mathbf{C}_1$, we have no pivot, except in a trivial sense, and hence, that the diagonal elements of $D^j(C)$ for all $\mathbf{C}$ (except E of course) must all be zero. An example of this type of structure can be seen for the representation E of $\mathbf{C}_{3v}$ (see table 3).

Clearly not all representations that one can write will have the simple structure described, because a unitary transformation will generally destroy it. This is the case, for instance, when one obtains a real representation for the representation E of $\mathbf{C}_{3v}$ just mentioned. Nevertheless, the fact that representations exist which have the simple structure described before has important consequences (see § 7).

6. The k vector

We shall now write down the representations $D^k(N)$ in a more explicit way, and we shall introduce an artifact, the **k** vector, that allows us to visualize very simply these representations and hence to simplify the various operations described in § 5 for reducing a group.

The n irreducible representations of a cyclic group $\mathbf{C}_n$ of order n are, as is well known, (see, for instance, Altmann 1962, p. 158)

$$D^k(C_r) = \exp\{\mathrm{i}(2\pi/n)\,kr\} \quad (k, r = 1, 2, \ldots, n). \tag{22}$$

A representation of a direct product of l cyclic groups will be denoted by a multiple index $k_1 k_2 \ldots k_l$ and is given by

$$D^{k_1 k_2 \ldots k_l}(C_{r_1} C_{r_2} \ldots C_{r_l}) = \exp \mathrm{i}\left(\frac{2\pi}{n_1} k_1 r_1 + \frac{2\pi}{n_2} k_2 r_2 + \ldots + \frac{2\pi}{n_l} k_l r_l\right). \tag{23}$$

In order to write (23) more compactly we introduce, as a mathematical artifact, two vectors $\mathbf{k} = k_1\boldsymbol{\kappa}_1 + k_2\boldsymbol{\kappa}_2 + \ldots + k_l\boldsymbol{\kappa}_l$ and $\mathbf{r} = r_1\boldsymbol{\tau}_1 + r_2\boldsymbol{\tau}_2 + \ldots + r_l\boldsymbol{\tau}_l$, where $|\boldsymbol{\kappa}_i| = 1$ and $|\boldsymbol{\tau}_i| = 2\pi/n_i$ for $i = 1, 2, \ldots, l$. Also, we impose the orthogonality condition

$$\boldsymbol{\kappa}_i \cdot \boldsymbol{\tau}_j = \delta_{ij}\, 2\pi/n_i. \tag{24}$$

Then, we can rewrite (23) as follows

$$D^{\mathbf{k}}(C_{\mathbf{r}}) = \mathrm{e}^{\mathrm{i}\,\mathbf{k}\cdot\mathbf{r}}. \tag{25}$$

A very well-known example of this is the translation subgroup of a space group, which is a direct product of cyclic groups when the Born–von Karman periodic conditions are used. The vector $\mathbf{r}$ here can be identified with a translation of the lattice. As the vectors $\boldsymbol{\tau}_1, \boldsymbol{\tau}_2, \ldots, \boldsymbol{\tau}_l$ (which are taken along the primitive axes of the crystal) are not in general orthogonal, the vectors $\boldsymbol{\kappa}_1, \boldsymbol{\kappa}_2, \ldots, \boldsymbol{\kappa}_l$ must be defined as unit vectors of the reciprocal lattice in order to verify the orthogonality condition (24) and the vector **k** which denotes the representation can be easily described as a reciprocal lattice vector.

This interpretation of (25) can be extended for the case when the group $\mathbf{C}_n$ is one of rotations around an n-fold axis. However, there are two important differences to be noted in this case. As we have seen, the introduction of the **k** vector is particularly valuable in dealing with direct product groups. Now if $\mathbf{C}_n$ and $\mathbf{C}_m$ are groups of rotations about two different axes the condition for their products to form a direct product group is that every C_n commutes with every C_m: this happens only in a most exceptional case, namely, when the rotation axes are perpendicular and the rotations binary. This is in fact the case for the two binary axes of $\mathbf{D}_2$: besides **T** which will be treated later, this is the only non-cyclic invariant subgroup that we have to consider, and so this stringent restriction does not, fortunately, prevent the use of the **k** vector in our case. In fact, because the rotation axes are orthogonal, it is not even necessary to introduce a reciprocal space: our **k** vector will be defined in the same space as the **r** vector. The vectors $\boldsymbol{\tau}_i$ which correspond to the rotation by $2\pi/n_i$ around the axis i, will be defined as *axial* vectors positive for counterclockwise rotations, parallel to the rotation axes and of length $|\boldsymbol{\tau}_i| = 2\pi/n_i$. Accordingly the $\boldsymbol{\kappa}_i$ will be *axial* unit vectors parallel to the $\boldsymbol{\tau}_i$. It should of course be clearly understood that this vector representation of finite rotations is only valid because we restrict ourselves to the case when the rotations commute. As regards the second difference to be made in dealing with rotations, we have already allowed for it: if a vector is to represent a rotation at all it must be an axial vector: it should be particularly remembered that an axial vector changes sign when it is reflected on a plane parallel to it.

It might be thought that the concept of a **k** vector would break down for the group **T**, and indeed it would fail in general, because the rotations around the threefold axis do not commute with those around the binary axes. Nevertheless, there are two cases for which this commutation is valid: when the rotation around the threefold axis is the identity (rotation by 2π) and when the rotations around the binary axes are the identity rotations. Trivial as these cases are, they are the only ones that appear in practice, and this allows us to denote the irreducible representations of **T** by a **k**-vector, as will be shown in § 8 (*b*).

A practical detail which should be noticed concerns the labelling of the components k_i of the **k** vector. In accordance with (22) $k_i = 1, 2, \ldots, n_i$, and a multiple of n_i can always be added to k_i. It is more convenient to symmetrize this interval, that is, if n_i is even, say, to take $k_i = -\frac{1}{2}n_i, \ldots, \frac{1}{2}n_i$, and similarly for n_i odd.

The **k** vectors allow us to obtain very quickly the star of a representation and, therefore its little group. Given a representation $D^{\mathbf{k}}(N)$ its star is given by the representations $\mathscr{C}D^{\mathbf{k}}(N)$, for $\mathscr{C}$ in **C**. Now $\mathscr{C}D^{\mathbf{k}}(N) = D^{\mathbf{k}}(\hat{C}^{-1}N)$ and if N is identified with C_r, this is the same as to write $\mathbf{k}.\hat{C}^{-1}\mathbf{r}$ in the exponent that appears on the right-hand side of (25). Because the operators concerned are unitary $\mathbf{k}.\hat{C}^{-1}\mathbf{r} = \hat{C}\mathbf{k}.\mathbf{r}$; that is, in order to form the conjugate representation of $D^{\mathbf{k}}$ under $\mathscr{C}$ it is enough to find the representation for which **k** takes the value $\hat{C}\mathbf{k}$. (When interpreting this latter symbol, remember that $\hat{C}\mathbf{k}$ is the value of **k** when the axes have been transformed by the operation C.)

In order to show how this work is carried out in practice we shall consider the group $\mathbf{C}_{3v} = \mathbf{C}_3 \wedge \mathbf{C}'_s$, where $\mathbf{C}'_s = E + \sigma_v$, and σ_v is a mirror plane that contains the rotation axis of $\mathbf{C}_3$. First, the **k** vectors and representations of $\mathbf{C}_3$: the unit vector $\boldsymbol{\kappa}$ will be parallel to the threefold axis and the **k** vectors will be -1, 0, 1, in units of κ, as follows from the (symmetrized) range for **k** given in (22). The star of $\mathbf{k} = -1$ is $E(-1) = -1$ and $\sigma_v(-1) = 1$; the co-group of **k** for this star is the identity because no operation of $\mathbf{C}_s$ leaves a **k** of the star invariant. The star of $\mathbf{k} = 0$ is clearly made up of the representation $\mathbf{k} = 0$ only: its co-group of **k** is now $\mathbf{C}_s'$. (Notice that the groups of **k** are, for the two stars given, $\mathbf{C}_3$ and $\mathbf{C}_{3v}$, respectively, but, of course, as explained in § 5(*c*), we do not require them in this case, since $\mathbf{C}_3$ is Abelian).

We next require the representations of the co-groups of **k** ($\mathbf{C}_1 = E$ and $\mathbf{C}_s$) and of $\mathbf{C}_3$. The representations of $\mathbf{C}_s$ are

$$\left.\begin{array}{ccc} \mathbf{C}_s & E & \sigma_v \\ A' & 1 & 1 \\ A'' & 1 & -1 \end{array}\right\} \tag{26}$$

Those of $\mathbf{C}_3$ are derived from (22) and are given in the left of table 3.

TABLE 3. THE REPRESENTATIONS OF $\mathbf{C}_{3v}$ IN RELATION TO THOSE OF $\mathbf{C}_3$

C_3 is a counterclockwise rotation by $\frac{2}{3}\pi$. $C_3\sigma_v$ and $C_3^2\sigma_v$ are mirror planes that form angles of $\frac{2}{3}\pi$ and $-\frac{2}{3}\pi$ respectively with σ_v.

$\epsilon = \exp(\frac{2}{3}\pi i)$

$\mathbf{C}_3$				E	C_3	C_3^2	$\mathbf{C}_{3v}$	E	C_3	C_3^2	σ_v	$C_3\sigma_v$	$C_3^2\sigma_v$
	k \ **r**			0	1	2	—	—	—	—	—	—	—
			co-group of **k**										
							A_1	1	1	1	1	1	1
A_1	0	star	$\mathbf{C}_s$	1	1	1							
							A_2	1	1	1	-1	-1	-1
^1E	1	star	$\mathbf{C}_1$	1	ϵ	ϵ^*	E	$\begin{bmatrix}1 & \\ & 1\end{bmatrix}$	$\begin{bmatrix}\epsilon & \\ & \epsilon^*\end{bmatrix}$	$\begin{bmatrix}\epsilon^* & \\ & \epsilon\end{bmatrix}$	$\begin{bmatrix} & 1\\ 1 & \end{bmatrix}$	$\begin{bmatrix} & \epsilon\\ \epsilon^* & \end{bmatrix}$	$\begin{bmatrix} & \epsilon^*\\ \epsilon & \end{bmatrix}$
^2E	-1			1	ϵ^*	ϵ							

An irreducible representation of $\mathbf{C}_{3v}$ will be fully determined by the star from $\mathbf{C}_3$ and one representation (the small representation) of the co-group of the **k** vector of the star. Because the group of A_1 ($\mathbf{k} = 0$) is $\mathbf{C}_s$, A_1 of $\mathbf{C}_3$ will produce two irreducible representations of $\mathbf{C}_{3v}$, in which the representatives of σ_v, from (26), are $+1$ and -1, respectively. Those of the remaining operations of $\mathbf{C}_{3v}$ are most simply obtained from the law of formation of the group as a product of $\mathbf{C}_3$ and $\mathbf{C}_s$. The representations ^1E and ^2E of $\mathbf{C}_3$ are joined together in the same star, with $\mathbf{C}_1$ as co-group of **k**, so that they will form just one two-dimensional representation of $\mathbf{C}_{3v}$. The matrices for the subgroup $\mathbf{C}_3$ of $\mathbf{C}_{3v}$ must be diagonal as shown in the table, because if ϕ_1 and ϕ_{-1} are bases of ^1E and ^2E, respectively,

$$C_3\langle\phi_1, \phi_{-1}| = \langle\epsilon\phi_1, \epsilon^*\phi_{-1}|$$

as follows from the representations of $\mathbf{C}_3$. In order to determine the remaining matrices it is enough, as before, to determine that for σ_v. This follows immediately because

$$\sigma_v\langle\phi_1, \phi_{-1}| = \langle\phi_{-1}, \phi_1|.$$

It is often desirable to obtain representations in real form, rather than the complex one shown in table 3 for $\mathbf{C}_{3v}$. This can be easily accomplished by a unitary transformation, such as that given by Altmann (1957*a*, p. 354).

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7. The bases of the representations

It is well known (see, for instance, Altmann 1962), that if we possess the representations of a group **G**, the operators

$$W^i_{tu} \equiv \sum_r D^i(G_r)^*_{tu} G_r \tag{27}$$

constructed from them are such that they transform an arbitrary function ϕ into another one ϕ^i_t—which following Melvin (1956) we shall call a symmetry-adapted function—that belongs to the tth column of the ith irreducible representation of **G**:

$$W^i_{tu}\phi = \phi^i_t. \tag{28}$$

If l_i is the dimensionality of the ith representation the suffix u in (27) and (28) can take any of the values $1, 2, \ldots, l_i$.

Another important relation for these operators is the following

$$W^i_{tu}\phi^j_v = \phi^i_t \delta_{ij}\delta_{uv}. \tag{29}$$

When $\mathbf{G} = \mathbf{N} \wedge \mathbf{C}$, we shall show that considerable simplification in the use of the operators (27) can be achieved by solving the problem stepwise: we first use (28), with the operators that correspond to **N**, to obtain functions that are symmetry adapted with respect to it. When these functions are themselves introduced in (28), now for the full group **G**, a simpler expression is obtained.

We can write $\mathbf{G} = \sum_i \mathbf{N}C_i$, and then

$$\begin{aligned} W^j_{tt} &= \sum_i \sum_s D^j(N_s C_i)^*_{tt} N_s C_i \\ &= \sum_i \sum_s D^j(C_i N_s)^*_{tt} C_i N_s. \end{aligned} \tag{30}$$

Here, in the second step, we can commute C_i and N_s because, on account of the invariance of **N**, both summations will cover exactly the same elements, except for the order. We can now express $D^j(C_i N_s)_{tt}$ by means of the standard matrix multiplication rule

$$\begin{aligned} W^j_{tt} &= \sum_i \sum_{su} D^j(C_i)^*_{tu} D^j(N_s)^*_{ut} C_i N_s \\ &= \sum_i \sum_u D^j(C_i)^*_{tu} C_i \sum_s D^j(N_s)^*_{ut} N_s. \end{aligned} \tag{31}$$

We know that the matrices $D^j(N)$ will be direct sums of matrices of irreducible representations of **N**, all derived star-wise from a given one $D^k(N)$. This means that the summation over s in (31) forms an operator like (27), for the group **N**. Now, we assumed that we have bases for this latter group, which for simplicity we shall label ϕ^j_t although different values of t may clearly belong to different representations of **N**. We operate with W^j_{tt} as given by (31) on ϕ^j_t: from (29) the summation over s gives ϕ^j_u, whence

$$W^j_{tt}\phi^j_t = \sum_u \sum_i D^j(C_i)^*_{tu} C_i \phi^j_u. \tag{32}$$

It should be carefully noticed that ϕ^j_t here is *not* a function that belongs to the jth representation of **G**: nevertheless, the left-hand side of (32) must be one such function on account of (28). This is obtained by projecting over the subgroup **C** the functions that belong to all the columns of the representation of **N** subduced by $D^j(G)$, and adding them up. If

n is the order of **N** and m that of **C** it is clear that we require to consider only $n+m$ matrices in the whole stepwise procedure, rather than $n.m$ (order of **G**) in the direct one.

The use of (32) can often be considerably simplified by bearing in mind the structure of the representations, as described in § 5 (d). We know that, when t is the column corresponding to the pivot of the representation the matrix elements $D^j(C_i N_s)_{tt}$ vanish whenever $C_i \notin \bar{\mathbf{K}}$. This means that in (30) and therefore in (32) we must add only over the operations $C_i \in \bar{\mathbf{K}}$. If $\bar{\mathbf{K}}$ is $\mathbf{C}_1$ every column can be considered a pivot and we have to add in (32) over the identity only: *the bases of* **N** *are taken over unchanged for* **G**.

If $\bar{\mathbf{K}} = \mathbf{C}_2$ or $\mathbf{C}_s$ the functions which are not pivots are such that for them $D^j(C_i N_s)_{tt} = 0$ for all C_i: hence the *non-pivotal functions of the basis of* **N** *are unchanged when going over to the group* **G**, *and the pivot has to be projected over* $\bar{\mathbf{K}}$. These results are valid only when $D^j(N)$ is diagonal and does not contain repeated representations of **N**. This is by far the most common case, and the rules given can be easily adapted for the case when $D^j(N)$ is not diagonal.

Although the application of these rules would anyhow be self-evident if a representation such as that displayed in table 3 for E of $\mathbf{C}_{3v}$ were used, it must be understood that these rules still obtain for any other, similar, representation, such as the well-known real one (see, for instance, Altmann & Bradley 1962) even though for the latter the cancellation of matrix elements described here does not take place. It is indeed for representations of this kind that the greatest benefit is derived from our rules, owing to the large number of non-vanishing matrix elements that such representations contain.

As an example, we shall consider $\mathbf{C}_{3v} = \mathbf{C}_3 \wedge \mathbf{C}_s$. We shall start from bases for $\mathbf{C}_3$ and we shall take them, as in the rest of this article, to be spherical harmonics both because these are the most natural functions to use as bases for the representations of the rotation group, and because there exists a considerable body of results for these functions (see Altmann 1957a, and Altmann & Bradley 1962). For simplicity we shall use unnormalized spherical harmonics

$$\mathscr{Y}_l^m(\theta,\phi) = P_l^m(\cos\theta)\,e^{im\phi}, \tag{33}$$

as well as their real forms

$$\mathscr{Y}_l^{m,c}(\theta,\phi) = P_l^m(\cos\theta)\cos m\phi, \tag{34}$$

$$\mathscr{Y}_l^{m,s}(\theta,\phi) = P_l^m(\cos\theta)\sin m\phi. \tag{35}$$

The bases for $\mathbf{C}_3$ are very easily obtained and they are given by Altmann (1957a, 1962). We follow the latter reference, where the notation agrees exactly with that of table 3.

The bases for A of $\mathbf{C}_3$ are all the harmonics $\mathscr{Y}_l^m$ with $m = 0$, mod 3. The bases for A_1 and A_2 of $\mathbf{C}_{3v}$ will therefore be, from (32),

$$\mathscr{Y}_l^m \pm \sigma_v \mathscr{Y}_l^m, \tag{36}$$

respectively, where the $\pm$ sign corresponds to the two representations of $\mathbf{C}_s$ listed in (26), and σ_v stands for a mirror plane parallel to the axis of $\mathbf{C}_3$. The transformation of the spherical harmonics under proper or improper rotations is well known and will not be described here (see Altmann 1957a). We write $\sigma_v = iC_2'$, where C_2' is a binary rotation perpendicular to the C_3 axis and i the inversion. In order to transform the harmonics we require the Euler angles of the rotation C_2. They are $\alpha = 0$, $\beta = \pi$, $\gamma = 0$ and therefore, from equation (29) of Altmann (1957a) we have $\sigma_v \mathscr{Y}_l^m = \mathscr{Y}_l^{-m}$. On introducing this result in (36) we find that the bases for A_1 and A_2 of $\mathbf{C}_{3v}$ are respectively $\mathscr{Y}_l^{m,c}$ and $\mathscr{Y}_l^{m,s}$, with m in every case equal to 0, mod + 3. (We write mod + 3, in an obvious notation, to stress the fact that no new function results when a negative m is taken.)

The group $\bar{\mathbf{K}}$ for E of $\mathbf{C}_{3v}$ is $\mathbf{C}_1$. Hence, we can simplify (32) or rather avoid its use entirely in this case by means of the rules given above: the bases of ${}^1E$ and ${}^2E$ of $\mathbf{C}_3$, which are $\mathscr{Y}_l^m$, $\mathscr{Y}_l^{-m}$, $m = 1 \bmod 3$, are straight away bases for E. They can be written as the row vector $\langle \mathscr{Y}_l^m, \mathscr{Y}_l^{-m} |$.

8. $\mathbf{D}_2$ AND THE CUBIC GROUPS

We shall apply in this section the whole theory that we have developed, now for a family of point groups: besides providing a useful example of the theory, this treatment will show how the method allows us to relate several point groups.

(a) *The group* $\mathbf{D}_2$

From table 2, $\mathbf{D}_2 = \mathbf{C}_2 \times \mathbf{C}_2'$, where the two binary axes are perpendicular. To indicate this fact most simply we shall change the notation. Define $\mathbf{C}_{2x} = E + C_{2x}$, $\mathbf{C}_{2y} = E + C_{2y}$ and then $\mathbf{D}_2 = \mathbf{C}_{2x} \times \mathbf{C}_{2y}$, where C_{2x} and C_{2y} are mutually perpendicular. Being a direct product, the representations of $\mathbf{D}_2$ are obtained by elementary methods: we shall derive them here only to identify the $\mathbf{k}$ vectors of the representations. The representations of $\mathbf{C}_{2x}$ and $\mathbf{C}_{2y}$ can be immediately written

$\mathbf{C}_{2x}$	$\mathbf{k}_x$	E	C_{2x}	$\mathbf{C}_{2y}$	$\mathbf{k}_y$	E	C_{2y}	
A	0	1	1	A	0	1	1	(37)
B	1	1	−1	B	1	1	−1	

Here, the values of $\mathbf{k}$ follow immediately from (22). The direct product is given by $\mathbf{D}_2 = E + C_{2x} + C_{2y} + C_{2z}$ with $C_{2z} = C_{2x}C_{2y}$, a binary axis perpendicular to the other two. When forming the representations for $\mathbf{D}_2$ those of $\mathbf{C}_{2x}$ and $\mathbf{C}_{2y}$ are combined in the standard manner, and we have a two-component $\mathbf{k}$ vector, the first and second component corresponding respectively to the value of $\mathbf{k}_x$ and $\mathbf{k}_y$ obtained from (37). These representations are given in table 4.

TABLE 4. REPRESENTATIONS AND BASES (SPHERICAL HARMONICS) FOR $\mathbf{D}_2$

$\mathbf{D}_2$	$\mathbf{k}$	E	C_{2x}	C_{2y}	C_{2z}	l	m mod(+2)	
A_1	(00)	1	1	1	1	0 3	0 2	c s
B_3	(01)	1	1	−1	−1	2 1	1 1	s c
B_2	(10)	1	−1	1	−1	2 1	1 1	c s
B_1	(11)	1	−1	−1	1	2 1	2 0	s c

In the last three columns of table 4 we specify, for future reference, the spherical harmonics, given by Altmann (1957*a*), that span the irreducible representations. These columns give the permitted values of l and m, and the superscripts c and s that appear in (34) and (35). In every case +2 can be added to m, as indicated, as well as to l.

It should be noticed that the two-dimensional $\mathbf{k}$ vector can sometimes be more easily visualized through a three-dimensional one, the third (redundant) component corresponding to z. In this notation (11) = (001) as follows from the relation $C_{2x}C_{2y} = C_{2z}$.

(b) *The group* $\mathbf{T}$

From table 2, $\mathbf{T} = \mathbf{D}_2 \wedge \mathbf{C}_3$ where the axis C_3 of $\mathbf{C}_3$ must be taken along the diagonal of the positive octant formed by the x, y, z axes of $\mathbf{D}_2$. We first find the stars of the representations of $\mathbf{T}$: (00) (of $\mathbf{D}_2$) will be a star on its own and its co-group is $\mathbf{C}_3$. The star of (01) will result from the axes transformations $C_3^+(xyz) = (yzx)$, $C_3^-(xyz) = (zxy)$. Hence

$$C_3^+(01) = (001) \equiv (11)$$

(this involves nothing more than to recognize that $C_3^+ y = z$) and $C_3^-(01) = (10)$. That is, (01), (10) and (11) form one star, the co-group of which is $\mathbf{C}_1$, the identity.

As $\mathbf{C}_3$ is the co-group of the star of (00), we require its representations, as well as those of $\mathbf{D}_2$, in order to obtain the representations of $\mathbf{T}$. They are given in table 5 and those of $\mathbf{D}_2$ in table 4.

TABLE 5. THE REPRESENTATIONS OF $\mathbf{C}_3$

$\epsilon = \exp(\frac{2}{3}\pi i)$

$\mathbf{C}_3$	$\mathbf{k}$	E	C_3^+	C_3^-
A	0	1	1	1
^1E	1	1	ϵ	ϵ^*
^2E	2	1	ϵ^*	ϵ

The star of (00) (co-group $\mathbf{C}_3$) will produce three one-dimensional representations, one for each of the representations of $\mathbf{C}_3$. Their derivation is now obvious. The star of (01), which is three-dimensional and has $\mathbf{C}_1$ for its group, will give one representation.

The matrices of the operations of $\mathbf{T}$ that belong to $\mathbf{D}_2$ are, as we know, direct sums of the representations of $\mathbf{D}_2$ that correspond to the star. That for C_{2x}, for instance, will be

$$\begin{bmatrix} 1 & & \\ & -1 & \\ & & -1 \end{bmatrix}. \tag{38}$$

The matrices for the operations of $\mathbf{T}$ not in $\mathbf{D}_2$ must have vanishing diagonal elements, because we have no pivot, the group of the star being $\mathbf{C}_1$ (see § 5 (d)). Hence their characters must vanish. We give the characters of the representations of $\mathbf{T}$ in table 6.

TABLE 6. THE CHARACTERS OF THE REPRESENTATIONS OF $\mathbf{T}$ AND THEIR RELATION TO $\mathbf{D}_2$

$\epsilon = \exp(\frac{2}{3}\pi i)$

$\mathbf{D}_2$	$\mathbf{k}(\mathbf{D}_2)$	co-group of $\mathbf{k}$	$\mathbf{T}$	$\mathbf{k}(\mathbf{T})$	E	$3C_2$	$4C_3^+$	$4C_3^-$	l mod (+2)	m mod (+2)	
			A	(00, 0)	1	1	1	1	—	—	—
A_1	(00)	$\mathbf{C}_3$ <	^1E	(00, 1)	1	1	ϵ	ϵ^*	—	—	—
			^2E	(00, 2)	1	1	ϵ^*	ϵ	—	—	—
B_3	(01)			(01, 0)					2	2	s
B_2	(10)	$\mathbf{C}_1$ >	T	[(10, 0)]	3	−1	0	0	1	0	c
B_1	(11)			[(11, 0)]					—	1	(c, s)

Two remarks must be made about the $\mathbf{k}$ symbols for $\mathbf{T}$ that appear in table 6. They cannot be regarded as three-dimensional vectors: the symbols on the left of the comma refer to the C_2 axes (as given for $\mathbf{D}_2$) and those to the right to the C_3 axis (as given for $\mathbf{C}_3$ in table 5). Operations about these different axes do not commute; the symbol is meaningless unless the $\mathbf{D}_2$ or the $\mathbf{C}_3$ parts of it vanish. This is in fact the case for those $\mathbf{k}$ 'vectors' in the table and they can therefore be used. Secondly, either of the three $\mathbf{k}$ vectors given for T is enough to denote fully this three-dimensional representation, and in order to stress this fact we give the redundant symbols in the table within square brackets. It is, nevertheless, useful to list all the partners in the star.

We shall now get in full the three-dimensional representation and its bases, which as always we take to be spherical harmonics. As regards the bases we know, because the co-group of the star is $\mathbf{C}_1$, that the bases of the representations of $\mathbf{D}_2$ that generate the star will be taken over unchanged for $\mathbf{T}$. We can read them off from table 4 and we collate the results in the last three columns of table 6. In the last line we use the symbol (c, s) for a pair $\langle \mathscr{Y}_l^{m,c}, \mathscr{Y}_l^{m,s}|$ that can be associated with any harmonic of the two previous lines to form a three-dimensional basis. No l value is given for this pair because l is arbitrary. To span the representation we can choose a basis from table 6. Take, for instance, $\langle \mathscr{Y}_1^{1,c}, \mathscr{Y}_1^{1,s}, \mathscr{Y}_1^0|$. The representation will be fully determined if we have the matrices for C_3^+ and C_3^-. In order to obtain them, it is enough to transform the harmonics under these operations. For the basis chosen this is trivial, as these harmonics have a very simple Cartesian representation. In a more general case recourse has to be taken to the method given by Altmann (1957*a*). The Euler angles for C_3^+ are $\alpha = 0$, $\beta = \frac{1}{2}\pi$, $\gamma = 0$. The transformation is effected by the following expression (see Altmann 1957*a*)

$$\mathscr{R}\mathscr{Y}_l^m = \sum_{m'} \mathscr{Y}_l^{m'} C_{m'm} \mathrm{e}^{\mathrm{i}m'\gamma} \mathrm{e}^{\mathrm{i}m\alpha} \mathscr{S}_{m'm}^{(l)}(\tfrac{1}{2}\pi). \tag{39}$$

Here $C_{m'm}$ can be either ± 1, and is tabulated in table 6 of that reference; $\mathscr{S}_{m'm}^{(l)}(\frac{1}{2}\pi)$ is tabulated up to $l = 6$ in table 10 of Altmann (1957*a*) and tables for it up to $l = 12$ have been computed (see Altmann & Bradley 1962). It is quickly found, in either way, that

$$C_3^+ \langle \mathscr{Y}_1^{1,c}, \mathscr{Y}_1^{1,s}, \mathscr{Y}_1^0| = \langle \mathscr{Y}_1^0, \mathscr{Y}_1^{1,c}, \mathscr{Y}_1^{1,s}|;$$

therefore the matrix is

$$D(C_3^+) = \begin{bmatrix} & 1 & \\ & & 1 \\ 1 & & \end{bmatrix}. \tag{40}$$

In the same manner $D(C_3^-)$ is obtained. The matrices of the operations that belong to $\mathbf{D}_2$ are obtained as in (38) and by multiplication the whole representation follows. It can be seen in full in table 7 of Altmann & Bradley (1962).

The derivation of the one-dimensional representations is trivial but not so that of their bases because the group is now $\mathbf{C}_3$. We have to project the bases for A_1 of $\mathbf{D}_2$ over $\mathbf{C}_3$. The general features of this projection can be quickly obtained because Altmann (1957*a*) has given, for any value l, m of an harmonic used as a generator of the expansion (28) a table that gives the values of l and m of the harmonics that will appear in the expansion. We know the possible generators for the required expansions, as they are read off from the two lines of table 4 that correspond to A_1. The values of l and m that will appear for these generators are now obtained from table 13·1 ($\mathbf{T}^{(2)}$) of the reference mentioned. They are given in table 7, for the representation A of $\mathbf{T}$.

The complete symmetry-adapted harmonics for A can be easily obtained by forming, from (32)

$$\mathscr{Y}_l^m + C_{31}^+ \mathscr{Y}_l^m + C_{31}^- \mathscr{Y}_l^m, \tag{41}$$

where $\mathscr{Y}_l^m$ must belong to A of $\mathbf{D}_2$. The transformations required in (41) are effected by means of (39): if we take $\mathscr{Y}_4^0$ as the generator we find that (41) assumes the form

$$\mathscr{Y}_4^0 + 2\mathscr{S}^{(4)}_{4,0}(\tfrac{1}{2}\pi)\,\mathscr{Y}_4^4 + 2\mathscr{S}^{(4)}_{4,0}(\tfrac{1}{2}\pi)\,\mathscr{Y}_4^{-4} + 2\mathscr{S}^{(4)}_{0,0}\,\mathscr{Y}_4^0 = \mathscr{Y}_4^0 + \tfrac{1}{168}\mathscr{Y}_4^{4,c}. \tag{42}$$

Here we obtained the symmetry-adapted harmonic in the right-hand side after replacing in the left the values of $\mathscr{S}^{(l)}_{m'm}(\frac{1}{2}\pi)$ obtained from the references mentioned.

TABLE 7. SPHERICAL HARMONICS FOR A OF $\mathbf{T}$

A single symmetrv-adapted spherical harmonic will be a linear combination of several of the functions listed below.

l mod (+2)	m mod (+4)	ϕ
0	0	c
3	2	s
6	2	c
9	4	s

(c) *The groups* $\mathbf{O}$ *and* $\mathbf{T}_d$

We shall use the expressions $\mathbf{O} = \mathbf{T} \wedge \mathbf{C}_2$ and $\mathbf{T}_d = \mathbf{T} \wedge \mathbf{C}_s$, where the C_2 axis bisects the first quadrant in the xy plane (defined as in $\mathbf{D}_2$ and $\mathbf{T}$) and the mirror σ_v of $\mathbf{C}_s$ contains both this C_2 axis and z. The stars and little co-groups of the representations, as well as the way in which they go from $\mathbf{D}_2$ to $\mathbf{O}$ and $\mathbf{T}_d$, are shown in table 8.

TABLE 8. THE RELATION BETWEEN THE REPRESENTATIVES OF $\mathbf{O}$ AND $\mathbf{T}_d$ AND THOSE OF $\mathbf{T}$

$\mathbf{T}$	$\mathbf{k}(\mathbf{T})$		little co-group $\mathbf{O}$	little co-group $\mathbf{T}_d$	representations of $\mathbf{O}$ or $\mathbf{T}_d$
A	(00, 0)	star	$\mathbf{C}_2$	$\mathbf{C}_s$	A_1, A_2
^1E ^2E	(00, 1) (00, 2)	star	$\mathbf{C}_1$	$\mathbf{C}_1$	E
T	(01, 0) [(10, 0)] [(11, 0)]	star	$\mathbf{C}_2$	$\mathbf{C}_s$	T_1, T_2

The details of the table should now be clear: it is enough to say that, for instance, (00, 1) and (00, 2) appear in the same star because C_2 and σ_v transform C_3^+ into C_3^- and hence (00, 1) into (00, 2) (see table 5). The actual form of the representations can now be readily obtained and will not be given here: they can be compared if necessary with the representations given by Altmann & Bradley (1962).

We shall show briefly how the bases of the one-dimensional representations are derived: we must form, from (32),

$$\mathscr{Y}_l^m + D(C)\,C\mathscr{Y}_l^m, \tag{43}$$

where $\mathscr{Y}_l^m$ must be one of the harmonics for A of $\mathbf{T}$ listed in table 7 and C is either C_2 or σ_v for $\mathbf{O}$ and $\mathbf{T}_d$, respectively. $D(C)$ will be unity for the totally symmetrical representation of $\mathbf{C}_2$ and $\mathbf{C}_s$ and -1 for the other. In order to obtain $C\mathscr{Y}_l^m$ we require the Euler angles of C_2 ($\alpha = 0$, $\beta = \pi$, $\gamma = \frac{1}{2}\pi$) and we must write $\sigma_v = iC_2'$ (binary rotation with Euler angles $\alpha = 0$, $\beta = \pi$ $\gamma = -\frac{1}{2}\pi$). Then, on using equation (29) of Altmann (1957*a*),

$$C_2\mathscr{Y}_l^m = (-1)^l\,\mathrm{e}^{-\frac{1}{2}\mathrm{i}m\pi}\,\mathscr{Y}_l^{-m}, \tag{44}$$

$$\sigma_v\mathscr{Y}_l^m = \mathrm{e}^{\frac{1}{2}\mathrm{i}m\pi}\,\mathscr{Y}_l^{-m}. \tag{45}$$

In these equations m can be positive or negative: accordingly, similar equations are obtained for $\mathscr{Y}_l^{m,c}$ and $\mathscr{Y}_l^{m,s}$. For instance, for the harmonics that appear in the second row of table 7, (43) gives:

$$\mathscr{Y}_3^{2,s} \mp D(C)\, \mathscr{Y}_3^{2,s}, \tag{46}$$

where the $-$ sign corresponds to **O** and the $+$ sign to $\mathbf{T}_d$. It is clear that this harmonic will vanish, for **O**, when $D(C) = 1$ and for $\mathbf{T}_d$ when $D(C) = -1$. Otherwise it will survive unchanged (except for an irrelevant factor). This means that this harmonic belongs to A_2 of **O** ($D(C) = -1$) and to A_1 of $\mathbf{T}_d$ ($D(C) = 1$). The remaining harmonics of table 7 are similarly treated: in every case they belong to one or the other of the representations A_1 and A_2. A complete table of this splitting is given by Altmann & Bradley (1962, table 4).

When we consider the three-dimensional representations, we meet for the first time a case where the representation $D^{\mathbf{k}}(N)$ of the invariant subgroup that generates the star is not one-dimensional. In fact, it is the three-dimensional representation T of **T**, which is the only representation that appears in the star. (This is clearly the case because this representation is invariant under the operations of $\mathbf{C}_2$ and also because it cannot be repeated since $\mathbf{C}_2$ is cyclic.) We can use very simply the result given at the end of § 5 (c). This means that a basis for T_1 or T_2 of **O** will be obtained by taking a basis for T of **T** such that one of its columns is either symmetrical or antisymmetrical with respect to C_2. The bases for T of **T** are given in table 6, and the column in question can be most conveniently chosen from the harmonics given in the first two lines for T. Their symmetry properties can be obtained by methods already fully described and will not now be repeated: if necessary they can be obtained from Altmann & Bradley (1962), where full tables for the representations can also be found.

The factorization $\mathbf{O} = \mathbf{T} \wedge \mathbf{C}_2$ fully describes, of course, the representations and bases of **O**. It might be useful, however, to consider briefly the factorization $\mathbf{O} = \mathbf{D}_2 \wedge \mathbf{D}_3$. If the axes of $\mathbf{D}_2$ are parallel to the edges of the cube, the $\mathbf{C}_3$ axis of $\mathbf{D}_3$ joins two opposite vertices of the cube and the three binary axes of $\mathbf{D}_3$ are the three, out of the six, binary axes that join opposite edges of the cube and that are perpendicular to the $\mathbf{C}_3$ axis chosen. If we refer to the representations of $\mathbf{D}_2$ we have two stars: (00) (co-group $\mathbf{D}_3$) and (01), (10) and (11) (co-group $\mathbf{C}_2$, where C_2 is the bisector of the first quadrant in the x, y plane in our standard set of axes). The representations of $\mathbf{D}_3$ are two one-dimensional (A_1 and A_2) and one two-dimensional (E) and it can be seen that the representations of **O** that are derived are the same as before. In particular the three-dimensional star will give two three-dimensional representations of **O**, T_1 and T_2, in accordance with the two irreducible representations of $\mathbf{C}_2$. In order to generate the star we take one function ϕ that belongs to, say, the symmetrical representation of $\mathbf{C}_2$ and to one of the representations of the star say (11) (see table 4). This will be the space Λ_1 of § 5 (c) and also the pivot of the representation. The other partners of the representation, that is the spaces Λ_2 and Λ_3 are obtained by acting on ϕ with the operations of $\mathbf{D}_3$ not in $\mathbf{C}_2$, that is with E, C_3^+, C_3^-. They must correspond to the other representations (10) and (01) of the star, just because these operations do not belong to its co-group. When this work is done, it will be found that $C_3^+\phi$ and $C_3^-\phi$ will belong to the antisymmetrical representation of $\mathbf{C}_2$ or, in general, to the one which is opposite to the representation of ϕ. We quote this result as an illustration of the situation mentioned in the footnote to page 228.

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The work reported in this and the preceding two papers has been made possible by a grant from the United Kingdom Atomic Energy Authority, which is gratefully acknowledged. The authors are grateful to Dr L. Fox for permission to use the facilities of the Computing Laboratory of the University of Oxford.

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