value since its occurrence provides a significant increase in the area of a crystal giving useful lattice images.

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Irreducible Representations of Point Groups

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The method of obtaining the irreducible representations of crystallographic point groups is discussed. It employs the little-group technique and makes use of the solvability property. Octahedral group **O** is treated as an illustration.

Introduction

Character tables for the 32 crystallographic point groups along with the methods of obtaining them are given extensively in several standard texts (Wilson, Decius & Cross, 1955). But the method of constructing the actual irreducible representations (IR's) which are useful for several practical applications is rarely discussed. In a classic paper dealing with the study of crystals, Bouckaert, Smoluchowski & Wigner (1936) have shown that the IR's of a space group can be obtained by using the allowable representations of the groups of wave vectors, known as little groups of the second kind. The details of this method have been explained very elegantly by Lomont (1959) and Bradley (1966).

In this note we shall discuss the construction of the IR's of any crystallographic point group (in fact of any solvable group) using the little-group method in conjunction with the solvability property (Lomont, 1959). Even though the application of the powerful little-group technique is strictly not necessary for point groups, it is instructive nevertheless to see how easily the actual representations can be obtained. As an illustration we shall consider the octahedral group **O**. also considered by Lomont in a somewhat different way. An application of the same method to the plane group *p*4*g* was considered by Raghavacharyulu (1961).

Since the method requires a certain amount of familarity with a number of terms, we shall first define them illustrating each with a relevant example. As an aid to the discussion, we shall refer to the character tables of the point groups $\mathbf{D}_2$, **T** and **O** and the quotient

Table 1. *Character table for the dihedral group* $\mathbf{D}_2$

$\mathbf{D}_2$	I	C_2^x	C_2^y	C_2^z
A	1	1	1	1
B_x	1	1	−1	−1
B_y	1	−1	1	−1
B_z	1	−1	−1	1

Generating elements: I, C_2^x, C_2^y

Defining relations: $(C_2^x)^2=(C_2^y)^2=I;\ C_2^yC_2^x\,C_2^y=C_2^x$

Table 2. *Character table for the tetrahedral group* **T**

T	I	$3C_2$	$4C_3$	$4C_3^2$
A	1	1	1	1
E_a	1	1	ϵ	ϵ^2
E_b	1	1	ϵ^2	ϵ
F	3	−1	0	0

$\epsilon=e^{2\pi i/3}$.

Generating elements: I, $C_3^{(1)}$, C_2^x

IR: F $\begin{pmatrix}1&0&0\\0&1&0\\0&0&1\end{pmatrix}$ $\begin{pmatrix}0&0&1\\1&0&0\\0&1&0\end{pmatrix}$ $\begin{pmatrix}1&0&0\\0&-1&0\\0&0&-1\end{pmatrix}$

Defining relations: $(C_2^x)^2=(C_3^{(1)})^3=I;(C_2^xC_3^{(1)})^2=C_2^x(C_3^{(1)})^2$

Table 3. *Character table for the octahedral group* **O**

O	I	$3C_2$	$8C_3$	$6C_4$	$6C_2'$
A_1	1	1	1	1	1
A_2	1	1	1	−1	−1
E	2	2	−1	0	0
F_1	3	−1	0	1	−1
F_2	3	−1	0	−1	1

Table 3 (*cont.*)

Generating elements:		I	C_4^x	$C_3^{(1)}$
	E	$\begin{pmatrix}1&0\\0&1\end{pmatrix}$	$\begin{pmatrix}0&1\\1&0\end{pmatrix}$	$\begin{pmatrix}\epsilon&0\\0&\epsilon^2\end{pmatrix}$
IR's:	F_1	$\begin{pmatrix}1&0&0\\0&1&0\\0&0&1\end{pmatrix}$	$\begin{pmatrix}1&0&0\\0&0&1\\0&-1&0\end{pmatrix}$	$\begin{pmatrix}0&0&1\\1&0&0\\0&1&0\end{pmatrix}$
	F_2	$\begin{pmatrix}1&0&0\\0&1&0\\0&0&1\end{pmatrix}$	$\begin{pmatrix}-1&0&0\\0&0&-1\\0&1&0\end{pmatrix}$	$\begin{pmatrix}0&0&1\\1&0&0\\0&1&0\end{pmatrix}$

Defining relations: $(C_4^x)^4=(C_3^{(1)})^3=I$; $[(C_4^x)^2=C_2^x]$; $C_4^x(C_3^{(1)})^2C_4^x=C_3^{(1)}$; $C_4^xC_3^{(1)}C_4^x=C_3^{(1)}(C_4^x)^2C_3^{(1)}$

Representation E can be transformed into one with real elements by subjecting it to the unitary transformation UEU^{-1} where $U=\frac{1}{\sqrt{2}}\begin{pmatrix}1&1\\i&-i\end{pmatrix}$.

group $\mathbf{T}/\mathbf{D}_2=\mathbf{C}_3$ given in Tables 1, 2, 3 and 4. The generating elements and the defining relations are also given below each table. The two generating elements of **O** are taken as C_4^x and $C_3^{(1)}$, the fourfold and threefold rotations, which transform a general point (xyz) into $(xz\bar{y})$ and (zxy) respectively. The transformation properties of (xyz) with respect to all the symmetry operations of **O** can be found in Henry & Lonsdale (1965). With the help of the defining relations, the group multiplication tables can easily be constructed. The group multiplication table for **O** is given, for instance, by Lomont (p. 33).

Table 4. *Character table for the quotient group* $\mathbf{T}/\mathbf{D}_2=\mathbf{C}_3$

$\mathbf{T}/\mathbf{D}_2=\mathbf{C}_3$	$\mathbf{D}_2$	$C_3^{(1)}\,.\,\mathbf{D}_2$	$(C_3^{(1)})^{-1}\,.\,\mathbf{D}_2$
A	1	1	1
$\begin{bmatrix}E_a\\E_b\end{bmatrix}$	1	ϵ	ϵ^2
	1	ϵ^2	ϵ

Definitions

In what follows, we shall assume that $\mathbf{G}=(A)$ is a finite group of order g and $\mathbf{H}=(B)$ is a normal subgroup of order h; A and B are typical elements of **G** and **H**; Δ an IR of **H** of dimension d and Γ a representation of **G**. $D^{\Gamma}(A)$ and $D^{\Delta}(B)$ are matrices representing elements A and B in the representations Γ and Δ.

Solvable group **G**

The series $\mathbf{G}=\mathbf{H}_0\supset\mathbf{H}_1\supset\mathbf{H}_2\ldots\supset\mathbf{I}$ in which $\mathbf{H}_{i+1}$ is a maximal normal subgroup of $\mathbf{H}_i$ is called a composition series of **G**; $\mathbf{H}_i/\mathbf{H}_{i+1}$ are called composition quotient groups and their orders h_i/h_{i+1} composition indices. **G** is a solvable group if its composition indices are prime numbers.

Example: $\mathbf{O}\supset\mathbf{T}\supset\mathbf{D}_2$ and the orders of $\mathbf{O}/\mathbf{T}$ and $\mathbf{T}/\mathbf{D}_2$ are 2 and 3. Thus **O** and hence **T** and $\mathbf{D}_2$ are solvable groups. In fact all groups of order less than 60 and hence all crystallographic point groups are solvable groups.

Conjugate representation Δ^A

A representation of **H** conjugate to Δ relative to **G** is defined by $\Delta^A\rightarrow D^{\Delta}(A\mathbf{H}A^{-1})$. In general Δ and Δ^A need not be equivalent ($\Delta\cdot\not\equiv\cdot\Delta^A$). But if they are, then Δ is said to be self-conjugate.

Example: In $\mathbf{D}_2$, the representation A is self-conjugate and B_x, B_y, B_z are conjugate but inequivalent to each other relative to **T**.

Little groups of the second and first kind $\mathbf{L}^{\mathrm{II}}$ *and* $\mathbf{L}^{\mathrm{I}}$

All the elements A of **G** for which $\Delta\cdot\equiv\cdot\Delta^A$ form the little group of the second kind relative to $\mathbf{G},\mathbf{H},\Delta$ and denoted by $\mathbf{L}^{\mathrm{II}}(\mathbf{G},\mathbf{H},\Delta)$. $\mathbf{L}^{\mathrm{II}}$ contains **H** as a maximal normal subgroup. The quotient group $\mathbf{L}^{\mathrm{I}}(\mathbf{G},\mathbf{H},\Delta)=\mathbf{L}^{\mathrm{II}}/\mathbf{H}$ is the corresponding little group of the first kind.

Example: $\mathbf{L}^{\mathrm{II}}(\mathbf{T},\mathbf{D}_2,A)=\mathbf{T}$ and $\mathbf{L}^{\mathrm{II}}(\mathbf{T},\mathbf{D}_2,B_x)=\mathbf{D}_2$; $\mathbf{L}^{\mathrm{I}}(\mathbf{T},\mathbf{D}_2,A)=\mathbf{T}/\mathbf{D}_2=\mathbf{C}_3$.

Orbit θ*

An orbit of a normal subgroup **H** of **G** is the maximal set of inequivalent IR's of **H** which are mutually conjugate relative to the elements of **G**. The number of IR's in θ is called the order of the orbit.

Examples: $\mathbf{D}_2$ has two orbits with respect to **T**: $\theta_1=A$; $\theta_2=\{B_x,B_y,B_z\}$. **T** has three orbits with respect to **O**: $\theta_1=A$; $\theta_2=\{E_a,E_b\}$; $\theta_3=F$.

Subduced representation $\Gamma^s=\Gamma\downarrow\mathbf{H}$

In the representation $\Gamma\rightarrow D^{\Gamma}(A)$ of **G**, those matrices $D^{\Gamma}(B)$ which are images of **H** form a representation of **H** called subduced representation and denoted by $\Gamma\downarrow\mathbf{H}=\Gamma^s\rightarrow D^{\Gamma}(B)$. It is of course of the same dimension as Γ and is in general reducible.

Examples: Let $\mathbf{G}=\mathbf{T}$ and $\mathbf{H}=\mathbf{D}_2$. $A\downarrow\mathbf{D}_2=A(\mathbf{D}_2)$; $E_a\downarrow\mathbf{D}_2=A(\mathbf{D}_2)$ and $F\downarrow\mathbf{D}_2=B_x\oplus B_y\oplus B_z$.

* Orbit, little groups of the second and first kind are sometimes called star, little group and little co-group respectively.

Induced representation $\Gamma \equiv \Delta^{\mathcal{G}} = \Delta \uparrow \mathbf{G}$

Let $\mathbf{G} = \sum_{i=1}^{g/h} A_i \mathbf{H}$ be a left coset decomposition of $\mathbf{G}$; $\sigma(A,B)$ a matrix of dimension g/h with elements

$$\sigma_{ij}(A,B) = 1 \text{ if } A_i B A_j^{-1} = A$$
$$= 0 \quad \text{otherwise;}$$

$D^{\Gamma}(A) = \sum_{B \in \mathbf{H}} \sigma(A,B) \otimes D^{\Delta}(B)$ where $\otimes$ and $\sum$ denote direct product and an ordinary matrix sum. Then $\Gamma \rightarrow D^{\Gamma}(A)$ is a representation of $\mathbf{G}$ of dimension $(g/h)d$ induced by Δ of $\mathbf{H}$ and denoted by $\Gamma = \Delta \uparrow \mathbf{G}$.

Example: Let $\mathbf{G} = \mathbf{T}$ and $\mathbf{H} = \mathbf{D}_2$. Taking C_2^x and $C_3^{(1)}$ as the generating elements of $\mathbf{T}$ and $\mathbf{T} = \mathbf{D}_2 + C_3^{(1)}\mathbf{D}_2 + (C_3^{(1)})^{-1}\mathbf{D}_2$, we have

$$D^{F}(I) = \sigma(I,I) \otimes D^{Bx}(I) = \begin{pmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 1 \end{pmatrix}$$

$$D^{F}(C_2^x) = \sigma(C_2^x, C_2^x) \otimes D^{Bx}(C_2^x) + \sigma(C_2^x, C_2^y) \otimes D^{Bx}(C_2^y) + \sigma(C_2^x, C_2^z) \otimes D^{Bx}(C_2^z)$$

$$= \begin{pmatrix} 1 & 0 & 0 \\ 0 & 0 & 0 \\ 0 & 0 & 0 \end{pmatrix} - \begin{pmatrix} 0 & 0 & 0 \\ 0 & 0 & 0 \\ 0 & 0 & 1 \end{pmatrix} - \begin{pmatrix} 0 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 0 \end{pmatrix} = \begin{pmatrix} 1 & 0 & 0 \\ 0 & -1 & 0 \\ 0 & 0 & -1 \end{pmatrix}$$

and

$$D^{F}(C_3^{(1)}) = \sigma(C_3^{(1)}, I) \otimes D^{Bx}(I) = \begin{pmatrix} 0 & 0 & 1 \\ 1 & 0 & 0 \\ 0 & 1 & 0 \end{pmatrix}.$$

Thus $F = B_x \uparrow \mathbf{T}$. The induced representation which for its actual form depends on the choice of the coset representatives A_i, nevertheless gives an equivalent representation for an alternative choice.

Engendered representation

A representation of $\mathbf{G}$ obtained from a representation of $\mathbf{G}/\mathbf{H}$ is called the engendered representation. If the representation of $\mathbf{G}/\mathbf{H}$ is irreducible, then so is the engendered representation.

Example: The three representations of the quotient group $\mathbf{T}/\mathbf{D}_2 = \mathbf{C}_3$, which is cyclic, are A, E_a, E_b and these are just the representations of $\mathbf{T}$ with the characters as shown in Table 2.

Allowable or small representation (AR) γ

γ is said to be an allowable representation of $\mathbf{L}^{\mathrm{II}}(\mathbf{G},\mathbf{H},\Delta)$ if γ subduces a multiple of Δ on $\mathbf{H}$, *i.e.* $\gamma \downarrow \mathbf{H} = m\Delta$.

Example: A, E_a and E_b are the three AR's of $\mathbf{L}^{\mathrm{II}}(\mathbf{T},\mathbf{D}_2,A) = \mathbf{T}$.

Key little-group theorem

If γ is an AR of $\mathbf{L}^{\mathrm{II}}(\mathbf{G},\mathbf{H},\Delta)$, then $\Gamma = \gamma \uparrow \mathbf{G}$ is irreducible and if the AR's of only one little group per orbit of $\mathbf{H}$ are used to induce the IR's of $\mathbf{G}$, then each IR of $\mathbf{G}$ is found once and only once. This theorem enables us to have a completely unambiguous classification of all the IR's of $\mathbf{G}$.

The method

The little-group technique of finding the IR's of $\mathbf{G}$ making use of the solvability property involves the following steps.

(i) Find the composition series $\mathbf{G} = \mathbf{H}_0 \supset \mathbf{H}_1 \supset \mathbf{H}_2 \ldots \supset \mathbf{I}$ for $\mathbf{G}$. Choosing $\mathbf{H} = \mathbf{H}_1$, we note that since $\mathbf{G}$ is a solvable group, the quotient group $\mathbf{G}/\mathbf{H}$ is a cyclic group of prime order $g/h = \alpha$, say and its representations are known.

(ii) Classify the IR's of $\mathbf{H}$ into orbits θ_i with respect to $\mathbf{G}$. The order of each orbit is either α_i or 1.

(iii) Choose one IR, say Δ_i of dimension d_i from each orbit θ_i. (*a*) If the order of θ_i is α_i, then $\mathbf{L}^{\mathrm{II}}(\mathbf{G},\mathbf{H},\Delta_i) = \mathbf{H}$ and there is only one IR of $\mathbf{G}$ of dimension $(g/h)d_i$ obtained by inducing with Δ_i. (*b*) If the order of θ_i is 1 and Δ_i is non-degenerate, there are α_i IR's of $\mathbf{G}$ which are engendered by the IR's of $\mathbf{G}/\mathbf{H}$. If Δ_i is degenerate, then the IR's of $\mathbf{G}$ are obtained from those of $\mathbf{G}/\mathbf{H}$ in conjunction with the defining relations for the generators of $\mathbf{G}$.

(iv) The IR's of $\mathbf{H} = \mathbf{H}_1$ are in turn obtained from those of $\mathbf{H}_2$ by repeating steps (ii) and (iii). In this way, one can reduce the problem of finding the IR's of a solvable group $\mathbf{G}$ to that of finding the composition series of $\mathbf{G}$ and that of finding the IR's of the cyclic groups.

Example

The method of finding the IR's of $\mathbf{O}$ is depicted in Fig. 1. Taking the composition series $\mathbf{O} \supset \mathbf{T} \supset \mathbf{D}_2$ for $\mathbf{O}$, we see that the quotient groups $\mathbf{O}/\mathbf{T}$ and $\mathbf{T}/\mathbf{D}_2$ are cyclic groups of prime orders 2 and 3. $\mathbf{D}_2$ has two orbits with

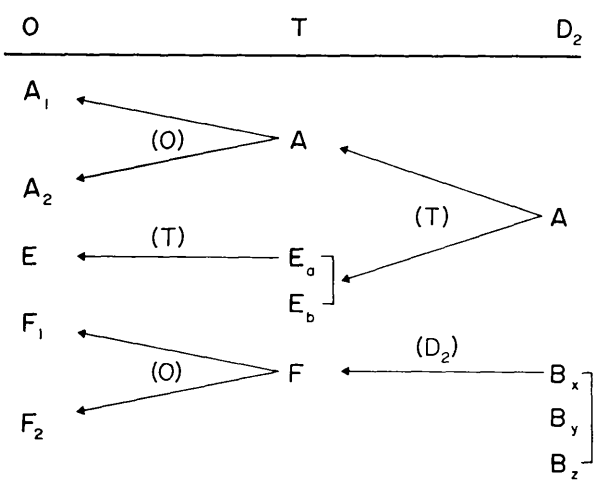

Fig. 1. Little-group technique of obtaining the IR's of $\mathbf{O}$ making use of the solvability property. The symbols within the parentheses represent little groups of the second kind $\mathbf{L}^{\mathrm{II}}(\mathbf{G},\mathbf{H},\Delta)$.

respect to **T**: $\theta_1 = A$ and $\theta_2 = \{B_x, B_y, B_z\}$. Thus there are three AR's of **T**, A, E_a, E_b, resulting from A and obtained by engendering with the IR's of $\mathbf{T}/\mathbf{D}_2 = \mathbf{C}_3$ and one three-dimensional representation F obtained by inducing with B_x. Obviously these AR's of **T** are themselves IR's of **T**.

The IR's of **T** are now classified into three orbits relative to **O**: $\theta_1 = A$, $\theta_2 = \{E_a, E_b\}$ and $\theta_3 = F$. Representation A gives rise to two IR's A_1, A_2 of **O** obtained by engendering with the IR's of $\mathbf{O}/\mathbf{T} = \mathbf{C}_2$ and E_a can be seen to induce the representation E. The two three-dimensional representations F_1, F_2 of **O** are obtained from F from the IR's of $\mathbf{O}/\mathbf{T} = \mathbf{C}_2$ and by noting that $(C_4^x)^2 = C_2^x$. The matrices thus obtained for the generating elements of the degenerate species of **T** and **O** are given below Tables 2 and 3.

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A Simple Direct Method for Solving Centrosymmetric Projections

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Fourier syntheses with a very few properly chosen terms can often represent structures quite well in projection. The use of triple-product relationships is shown to optimize the choice of terms for such a synthesis while minimizing the necessary number of sign combinations. The application of this method is demonstrated in the solutions of three structures: (1) 2,3-dimethoxybenzoic acid (orthoveratric acid); (2) (±)-2,4,6-trimethylpimelic acid; (3) morpholinium nitrate.

Several methods for solving crystal structures using only a very few structure factors have been put forward. These include Lonsdale's (1929) classic solution of hexamethylbenzene, Robertson's (1945) solution of coronene, and Woolfson's (1954) method of permutation syntheses. We wish to call attention to what we believe to be the optimal method of using a few structure factors, based on Cochran's (1952) discussion of the representation of electron density by Fourier series.

Lonsdale's method, used later by Robertson, depends on the recognition that if $|U_{hkl}|$ is near the maximum value of 1·0, then *all* the atomic centres must lie on or close to the crests of that Fourier component of the electron density. If there are several such U_{hkl}, what may be called geometrical Fourier summations can then be made, and a molecular model fit to those regions where crests coincide, the correct set of signs being found by trial and error. Figs. 1 and 2 show such syntheses for hexamethylbenzene and for coronene. Since, however, reflexions with $|U|$ near 1·0 usually arise from special structural features, they are generally quite rare, and without such outstandingly strong reflexions this method cannot be applied.

Woolfson's method of permutation syntheses is completely general, but has other severe limitations. The grounds for selection of terms included in the syntheses are left somewhat vague. The choice of signs is based not on any crystallographic information but solely on a combinatorial analysis. It is accepted in advance that one sign in seven may be wrong, in order to limit the number of combinations that need be tried, which even so is rather large (for example, 256 syntheses for 16 terms).

The method we propose relies first of all on the fact that, in projection down a reasonably short axis, the usual numerical Fourier summation made with quite a small number of properly chosen terms can be sufficient to reveal all or most of a structure. The terms should be chosen from the largest E's, as these in gen-

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