3

Character of a Representation

We have already discussed the arbitrariness of a representation with regard to similarity or equivalence transformations. Namely, if $D^{(\Gamma_j)}(R)$ is a representation of a group, so is $U^{-1}D^{(\Gamma_j)}(R)U$. To get around this arbitrariness, we introduce the use of the trace (or character) of a matrix representation which remains invariant under a similarity transformation. In this chapter we define the character of a representation, derive the most important theorems for the character, summarize the conventional notations used to denote symmetry operations and groups, and we discuss the construction of some of the most important character tables for the so-called point groups, that are listed in Appendix A. *Point groups* have no translation symmetry, in contrast to the *space groups*, that will be discussed in Chap. 9, and include both point group symmetry operations and translations.

3.1 Definition of Character

Definition 17. *The* character *of the matrix representation $\chi^{\Gamma_j}(R)$ for a symmetry operation R in a representation $D^{(\Gamma_j)}(R)$ is the* trace *(or the sum over diagonal matrix elements) of the matrix of the representation:*

$$\chi^{(\Gamma_j)}(R) = \mathrm{trace}\, D^{(\Gamma_j)}(R) = \sum_{\mu=1}^{\ell_j} D^{(\Gamma_j)}(R)_{\mu\mu}\,, \tag{3.1}$$

where ℓ_j is the dimensionality of the representation Γ_j and j is a representation index. From the definition, it follows that representation Γ_j will have h characters, one for each element in the group. Since the trace of a matrix is invariant under a similarity transformation, the character is invariant under such a transformation.

3.2 Characters and Class

We relate concepts of class (see Sect. 1.6) and character by the following theorem.

Theorem. *The character for each element in a class is the same.*

Proof. Let A and B be elements in the same class. By the definition of class this means that A and B are related by conjugation (see Sect. 1.6)

$$A = Y^{-1}BY\,, \tag{3.2}$$

where Y is an element of the group. Each element can always be represented by a unitary matrix D (see Sect. 2.4), so that

$$D(A) = D(Y^{-1})\,D(B)\,D(Y) = D^{-1}(Y)\,D(B)\,D(Y)\,. \tag{3.3}$$

And since a similarity transformation leaves the trace invariant, we have the desired result for characters in the same class: $\chi(A) = \chi(B)$, which completes the proof. □

The property that all elements in a class have the same character is responsible for what van Vleck called "the great beauty of character." If two elements of a group are in the same class, this means that they correspond to similar symmetry operations – e.g., the class of twofold axes of rotation of the equilateral triangle, or the class of threefold rotations for the equilateral triangle.

Sometimes a given group will have more than one kind of twofold symmetry axis. To test whether these two kinds of axes are indeed symmetrically inequivalent, we check whether or not they have the same characters.

We summarize the information on the characters of the representations of a group in the celebrated *character table*. In a character table we list the irreducible representations (IR) in column form (for example, the left-hand column of the character table) and the class as rows (top row labels the class). For example, the character table for the permutation group $P(3)$ (see Sect. 1.2) is shown in Table 3.1. (Sometimes you will see character tables with the columns and rows interchanged relative to this display.)

Table 3.1. Character table for the permutation group $P(3)$ or equivalently for group "D_3" (see Sect. 3.9 for group notation)

class → IR ↓	$\mathcal{C}_1$ $\chi(E)$	$3\mathcal{C}_2$ $\chi(A,B,C)$	$2\mathcal{C}_3$ $\chi(D,F)$
Γ_1	1	1	1
$\Gamma_{1'}$	1	−1	1
Γ_2	2	0	−1

Table 3.2. Classes for group "D_3" or equivalently for the permutation group $P(3)$ and for the symmetry operations of the equilateral triangle

notation for each class of	D_3	equilateral triangle	$P(3)$[a]
class 1 E ($N_k = 1$)	$1\mathcal{C}_1$	(identity class)	(1)(2)(3)
class 2 A, B, C ($N_k = 3$)	$3\mathcal{C}_2$	(rotation of π about twofold axis)	(1)(23)
class 3 D, F ($N_k = 2$)	$2\mathcal{C}_3$	(rotation of 120° about threefold axis)	(123)

[a]For the class notation for $P(3)$ see Chap. 17

We will see in Sect. 3.9 that this group, more specifically this *point* group is named D_3 (Schoenflies notation). In Table 3.1 the notation $N_k\mathcal{C}_k$ is used in the character table to label each class $\mathcal{C}_k$, where N_k is the number of elements in $\mathcal{C}_k$. If a representation is irreducible, then we say that its character is *primitive.* In a character table we limit ourselves to the primitive characters. The classes for group D_3 and $P(3)$ are listed in Table 3.2, showing different ways that the classes of a group are presented.

Now that we have introduced character and character tables, let us see how to use the character tables. To appreciate the power of the character tables we present in the following sections a few fundamental theorems for character.

3.3 Wonderful Orthogonality Theorem for Character

The "Wonderful Orthogonality Theorem" for character follows directly

from the wonderful orthogonality theorem (see Sect. 2.7). There is also a second orthogonality theorem for character which is discussed later (see Sect. 3.6). These theorems give the basic orthonormality relations used to set up character tables.

Theorem. *The primitive characters of an irreducible representation obey the orthogonality relation*

$$\sum_R \chi^{(\Gamma_j)}(R)\, \chi^{(\Gamma_{j'})}(R^{-1}) = h\delta_{\Gamma_j,\Gamma_{j'}} \tag{3.4}$$

or

$$\sum_R \chi^{(\Gamma_j)}(R)\, \chi^{(\Gamma_{j'})}(R)^* = h\delta_{\Gamma_j,\Gamma_{j'}}\ , \tag{3.5}$$

where Γ_j denotes irreducible representation j with dimensionality ℓ_j.

This theorem says that unless the representations are identical or equivalent, the characters are orthogonal in h-dimensional space, where h is the order of the group.

Example. We now illustrate the meaning of the Wonderful Orthogonality Theorem for characters before going to the proof. Consider the permutation group $P(3)$. Let $\Gamma_j = \Gamma_1$ and $\Gamma_{j'} = \Gamma_{1'}$. Then use of (3.13) yields

$$\sum_k N_k \chi^{(\Gamma_j)}(\mathcal{C}_k)\left[\chi^{(\Gamma_{j'})}(\mathcal{C}_k)\right]^* = \underbrace{(1)(1)(1)}_{\text{class of } E} + \underbrace{(3)(1)(-1)}_{\text{class of } A,B,C} + \underbrace{(2)(1)(1)}_{\text{class of } D,F}$$
$$= 1 - 3 + 2 = 0\,. \tag{3.6}$$

It can likewise be verified that the Wonderful Orthogonality Theorem works for all possible combinations of Γ_j and $\Gamma_{j'}$ in Table 3.1.

Proof. The proof of the wonderful orthogonality theorem for character follows from the Wonderful Orthogonality Theorem itself (see Sect. 2.7). Consider the wonderful orthogonality theorem (2.51)

$$\sum_R D_{\mu\nu}^{(\Gamma_j)}(R) D_{\nu'\mu'}^{(\Gamma_{j'})}(R^{-1}) = \frac{h}{\ell_j}\delta_{\Gamma_j,\Gamma_{j'}}\delta_{\mu\mu'}\delta_{\nu\nu'}\,. \tag{3.7}$$

Take the diagonal elements of (3.7)

$$\sum_R D_{\mu\mu}^{(\Gamma_j)}(R) D_{\mu'\mu'}^{(\Gamma_{j'})}(R^{-1}) = \frac{h}{\ell_j}\delta_{\Gamma_j,\Gamma_{j'}}\delta_{\mu\mu'}\delta_{\mu'\mu}\,. \tag{3.8}$$

Now sum (3.8) over μ and μ' to calculate the traces or characters

$$\sum_R \sum_\mu D_{\mu\mu}^{(\Gamma_j)}(R) \sum_{\mu'} D_{\mu'\mu'}^{(\Gamma_{j'})}(R^{-1}) = \frac{h}{\ell_j}\delta_{\Gamma_j,\Gamma_{j'}} \sum_{\mu\mu'} \delta_{\mu\mu'}\delta_{\mu'\mu}\,, \tag{3.9}$$

where we note that

$$\sum_{\mu\mu'} \delta_{\mu\mu'}\delta_{\mu'\mu} = \sum_\mu \delta_{\mu\mu} = \ell_j\,, \tag{3.10}$$

so that

$$\sum_R \chi^{(\Gamma_j)}(R)\chi^{(\Gamma_{j'})}(R^{-1}) = h\delta_{\Gamma_j,\Gamma_{j'}}\,, \tag{3.11}$$

completing the proof. Equation (3.11) implies that the primitive characters of an irreducible representation form a set of *orthogonal* vectors in *group-element* space, the space spanned by h vectors, one for each element of the group, also called Hilbert space (see Sect. 2.8). Since any arbitrary representation is equivalent to some unitary representation (Sect. 2.4), and the character is preserved under a unitary transformation, (3.11) can also be written as

$$\sum_R \chi^{(\Gamma_j)}(R)\left[\chi^{(\Gamma_{j'})}(R)\right]^* = h\delta_{\Gamma_j,\Gamma_{j'}}\,. \tag{3.12}$$

Since the character is the same for each element in the class, the summation in (3.12) can be written as a sum over classes k

$$\sum_k N_k \chi^{(\Gamma_j)}(\mathcal{C}_k) \left[\chi^{(\Gamma_{j'})}(\mathcal{C}_k)\right]^* = h\delta_{\Gamma_j,\Gamma_{j'}} , \tag{3.13}$$

where N_k denotes the number of elements in class k, since the representation for R is a unitary matrix, $\chi^{(\Gamma_{j'})}(R^{-1}) = [\chi^{(\Gamma_{j'})}(R)]^*$ (see Sect. 2.2). Also, since the right-hand side of (3.13) is real, we can take the complex conjugate of this equation to obtain the equivalent form

$$\sum_k N_k \left[\chi^{(\Gamma_j)}(\mathcal{C}_k)\right]^* \chi^{(\Gamma_{j'})}(\mathcal{C}_k) = h\delta_{\Gamma_j,\Gamma_{j'}} . \tag{3.14}$$

□

The importance of the results in (3.11)–(3.14) cannot be over-emphasized:

1. Character tells us if a representation is irreducible or not. If a representation is reducible then the characters are not primitive and will generally not obey this orthogonality relation (and other orthogonality relations that we will discuss in Sect. 3.6).
2. Character tells us whether or not we have found all the irreducible representations. For example, the permutation group $P(3)$ could not contain a three-dimensional irreducible representation (see Problem 1.2), since by (2.70)

$$\sum_j \ell_j^2 \le h . \tag{3.15}$$

Furthermore, character allows us to check the uniqueness of an irreducible representation, using the following theorem.

Theorem. *A necessary and sufficient condition that two irreducible representations be equivalent is that the characters be the same.*

Proof. Necessary condition: If they are equivalent, then the characters are the same – we have demonstrated this already since the trace of a matrix is invariant under an equivalence transformation.
Sufficient condition: If the characters are the same, the vectors for each of the irreducible representations in h-dimensional space cannot be orthogonal, so the representations must be equivalent. □

3.4 Reducible Representations

We now prove a theorem that forms the basis for setting up the characters of a *reducible* representation in terms of the primitive characters for the irreducible representations. This theoretical background will also be used in constructing irreducible representations and character tables, and is essential to most of the practical applications of group theory to solid state physics.

Theorem. *The reduction of any reducible representation into its irreducible constituents is unique.*

Thus, if $\chi(\mathcal{C}_k)$ is the character for some class in a reducible representation, then this theorem claims that we can write the character for the reducible representation $\chi(\mathcal{C}_k)$ as a linear combination of characters for the *irreducible* representations of the group $\chi^{(\Gamma_i)}(\mathcal{C}_k)$

$$\chi(\mathcal{C}_k) = \sum_{\Gamma_i} a_i \chi^{(\Gamma_i)}(\mathcal{C}_k)\,, \tag{3.16}$$

where the a_i coefficients are non-negative integers which denote the number of times the irreducible representation Γ_i is contained in the reducible representation. Furthermore we show here that the a_i coefficients are unique. This theorem is sometimes called the decomposition theorem for reducible representations.

Proof. In proving that the a_i coefficients are unique, we explicitly determine the values of each a_i, which constitute the characters for a reducible representation. Consider the sum over classes k:

$$\sum_k N_k \left[\chi^{(\Gamma_j)}(\mathcal{C}_k)\right]^* \chi(\mathcal{C}_k) = S_j\,. \tag{3.17}$$

Since $\chi(\mathcal{C}_k)$ is reducible, we write the linear combination for $\chi(\mathcal{C}_k)$ in (3.17) using (3.16) as

$$\begin{aligned} S_j &= \sum_k N_k \left[\chi^{(\Gamma_j)}(\mathcal{C}_k)\right]^* \sum_{\Gamma_i} a_i \chi^{(\Gamma_i)}(\mathcal{C}_k) \\ &= \sum_{\Gamma_i} a_i \left\{ \sum_k N_k \left[\chi^{(\Gamma_j)}(\mathcal{C}_k)\right]^* \chi^{(\Gamma_i)}(\mathcal{C}_k) \right\}\,. \end{aligned} \tag{3.18}$$

We now apply the Wonderful Orthogonality Theorem for Characters (3.13) to get

$$\sum_{\Gamma_i} a_i h \delta_{\Gamma_i,\Gamma_j} = a_j h = \sum_k N_k \left[\chi^{(\Gamma_j)}(\mathcal{C}_k)\right]^* \chi(\mathcal{C}_k) = S_j \tag{3.19}$$

yielding the decomposition relation

$$a_j = \frac{1}{h} \sum_k N_k \left[\chi^{(\Gamma_j)}(\mathcal{C}_k)\right]^* \chi(\mathcal{C}_k) = \frac{S_j}{h} \tag{3.20}$$

and completing the proof of the theorem. Thus the coefficients a_i in (3.16) are uniquely determined. In other words, the number of times the various irreducible representations are contained in a given reducible representation can be obtained directly from the character table for the group.

This sort of decomposition of the character for a reducible representation is important for the following type of physical problem. Consider a *cubic crystal*. A cubic crystal has many symmetry operations and therefore many classes and many irreducible representations. Now suppose that we squeeze this crystal and lower its symmetry. Let us further suppose that the energy levels for the cubic crystal are degenerate for certain points in the Brillouin zone. This squeezing would most likely lift some of the level degeneracies. To find out how the degeneracy is lifted, we take the representation for the cubic group that corresponds to the unperturbed energy and treat this representation as a reducible representation in the group of lower symmetry. Then the decomposition formulae (3.16) and (3.20) tell us immediately the degeneracy and symmetry types of the split levels in the perturbed or stressed crystal. (A good example of this effect is crystal field splitting, discussed in Chap. 5.) □

3.5 The Number of Irreducible Representations

We now come to another extremely useful theorem.

Theorem. *The number of irreducible representations is equal to the number of classes.*

Proof. The Wonderful Orthogonality Theorem for Character (3.14)

$$\sum_{k'=1}^{k} N_{k'} \left[\chi^{(\Gamma_i)}(\mathcal{C}_{k'})\right]^* \chi^{(\Gamma_j)}(\mathcal{C}_{k'}) = h\,\delta_{\Gamma_i,\Gamma_j} \tag{3.21}$$

can be written as

$$\sum_{k'=1}^{k} \left[\sqrt{\frac{N_{k'}}{h}}\,\chi^{(\Gamma_i)}(\mathcal{C}_{k'})\right]^* \left[\sqrt{\frac{N'_k}{h}}\,\chi^{(\Gamma_j)}(\mathcal{C}_{k'})\right] = \delta_{\Gamma_i,\Gamma_j}\,. \tag{3.22}$$

Each term

$$\sqrt{\frac{N_{k'}}{h}}\,\chi^{(\Gamma_i)}(\mathcal{C}_{k'})$$

in (3.22) gives the k'th component of a k-dimensional vector. There can be only k such vectors in a k-dimensional space, since the $(k+1)$th vector would be linearly dependent on the other k vectors. If there were less than k such vectors, then the number of independent vectors would not be large enough to span the k-dimensional space. To express a reducible representation in terms of its irreducible components requires that the vector space be spanned by irreducible representations. Therefore the number of irreducible representations must be k, the number of classes.

For our example of the permutation group of three objects, we have three classes and therefore only three irreducible representations (see Table 3.1). We have already found these irreducible representations and we now know that any additional representations that we might find are either *equivalent* to these representations or they are *reducible*. Knowing the number of distinct irreducible representations is very important in setting up character tables.

As a corollary of this theorem, the number of irreducible representations for Abelian groups is the number of symmetry elements in the group, because each element is in a class by itself. Since each class has only one element, all the irreducible representations are one dimensional. □

3.6 Second Orthogonality Relation for Characters

We now prove a second orthogonality theorem for characters which sums over the irreducible representations and is extremely valuable for constructing character tables.

Theorem. *The summation over all irreducible representations*

$$\sum_{\Gamma_j} \chi^{(\Gamma_j)}(\mathcal{C}_k) \left[\chi^{(\Gamma_j)}(\mathcal{C}_{k'})\right]^* N_k = h\delta_{kk'} \tag{3.23}$$

yields a second orthogonality relation for the characters. Thus, the Wonderful Orthogonality Theorem for Character yields an orthogonality relation between rows in the character table while the second orthogonality theorem gives a similar relation between the columns of the character table.

Proof. Construct the matrix

$$Q = \begin{pmatrix} \chi^{(1)}(\mathcal{C}_1) & \chi^{(1)}(\mathcal{C}_2) & \cdots \\ \chi^{(2)}(\mathcal{C}_1) & \chi^{(2)}(\mathcal{C}_2) & \cdots \\ \chi^{(3)}(\mathcal{C}_1) & \chi^{(3)}(\mathcal{C}_2) & \cdots \\ \vdots & \vdots & \end{pmatrix}, \tag{3.24}$$

where the irreducible representations label the rows and the classes label the columns. Q is a square matrix, since by (3.22) the number of classes (designating the column index) is equal to the number of irreducible representations (designating the row index). We now also construct the square matrix

$$Q' = \frac{1}{h}\begin{pmatrix} N_1\chi^{(1)}(\mathcal{C}_1)^* & N_1\chi^{(2)}(\mathcal{C}_1)^* & \cdots \\ N_2\chi^{(1)}(\mathcal{C}_2)^* & N_2\chi^{(2)}(\mathcal{C}_2)^* & \cdots \\ N_3\chi^{(1)}(\mathcal{C}_3)^* & N_3\chi^{(2)}(\mathcal{C}_3)^* & \cdots \\ \vdots & \vdots & \end{pmatrix}, \tag{3.25}$$

where the classes label the rows, and the irreducible representations label the columns. The ij matrix element of the product QQ' summing over classes is then

$$(QQ')_{ij} = \sum_k \frac{N_k}{h} \chi^{(\Gamma_i)}(\mathcal{C}_k) \left[\chi^{(\Gamma_j)}(\mathcal{C}_k)\right]^* = \delta_{\Gamma_i,\Gamma_j} \tag{3.26}$$

using the Wonderful Orthogonality Theorem for Character (3.13). Therefore $QQ' = \hat{1}$ or $Q' = Q^{-1}$ and $Q'Q = \hat{1}$ since $QQ^{-1} = Q^{-1}Q = \hat{1}$, where $\hat{1}$ is the unit matrix. We then write $Q'Q$ in terms of components, but now summing over the irreducible representations

$$(Q'Q)_{kk'} = \sum_{\Gamma_i} \frac{N_k}{h} \chi^{(\Gamma_i)}(\mathcal{C}_k) \left[\chi^{(\Gamma_i)}(\mathcal{C}_{k'})\right]^* = \delta_{kk'} \tag{3.27}$$

so that

$$\sum_{\Gamma_i} \chi^{(\Gamma_i)}(\mathcal{C}_k) \left[\chi^{(\Gamma_i)}(\mathcal{C}_{k'})\right]^* = \frac{h}{N_k}\delta_{kk'}\,, \tag{3.28}$$

which completes the proof of the second orthogonality theorem. □

3.7 Regular Representation

The regular representation provides a recipe for finding all the irreducible representations of a group. It is not always the fastest method for finding the irreducible representations, but it will always work.

The *regular representation* is found directly from the multiplication table by rearranging the rows and columns so that the identity element is always along the main diagonal. When this is done, the group elements label the columns and the inverse of each group element labels the rows. We will illustrate this with the permutation group of three objects $P(3)$ for which the multiplication table is given in Table 1.1. Application of the rearrangement theorem to place the identity element along the main diagonal gives Table 3.3. Then the matrix representation for an element X in the regular representation is obtained by putting 1 wherever X appears in the multiplication Table 3.3

Table 3.3. Multiplication table for the group $P(3)$ used to generate the regular representation

	E	A	B	C	D	F
$E = E^{-1}$	E	A	B	C	D	F
$A = A^{-1}$	A	E	D	F	B	C
$B = B^{-1}$	B	F	E	D	C	A
$C = C^{-1}$	C	D	F	E	A	B
$F = D^{-1}$	F	B	C	A	E	D
$D = F^{-1}$	D	C	A	B	F	E

and 0 everywhere else. Thus we obtain

$$D^{\mathrm{reg}}(E) = \begin{pmatrix} 1 & 0 & 0 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 & 0 & 0 \\ 0 & 0 & 1 & 0 & 0 & 0 \\ 0 & 0 & 0 & 1 & 0 & 0 \\ 0 & 0 & 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & 0 & 0 & 1 \end{pmatrix}, \tag{3.29}$$

which is always the unit matrix of dimension $(h \times h)$. For one of the other elements in the regular representation we obtain

$$D^{\mathrm{reg}}(A) = \begin{pmatrix} 0 & 1 & 0 & 0 & 0 & 0 \\ 1 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 1 \\ 0 & 0 & 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & 1 & 0 & 0 \\ 0 & 0 & 1 & 0 & 0 & 0 \end{pmatrix} \tag{3.30}$$

and so on. By construction, only $D^{\mathrm{reg}}(E)$ has a non-zero trace!

We now show that the regular representation is indeed a representation. This means that the regular representation obeys the multiplication table (either Table 1.1 or 3.3). Let us for example show

$$D^{\mathrm{reg}}(BC) = D^{\mathrm{reg}}(B) D^{\mathrm{reg}}(C)\,. \tag{3.31}$$

It is customary to denote the matrix elements of the regular representation directly from the definition $D^{\mathrm{reg}}(X)_{A_k^{-1},A_i}$, where A_k^{-1} labels the rows and A_i labels the columns using the notation

$$D^{\mathrm{reg}}(X)_{A_k^{-1},A_i} = \begin{cases} 1 & \text{if} \quad A_k^{-1} A_i = X \\ 0 & \text{otherwise}\,. \end{cases} \tag{3.32}$$

Using this notation, we have to show that

$$D^{\mathrm{reg}}(BC)_{A_k^{-1},A_i} = \sum_{A_j} D^{\mathrm{reg}}(B)_{A_k^{-1},A_j} D^{\mathrm{reg}}(C)_{A_j^{-1},A_i}\,. \tag{3.33}$$

Now look at the rearranged multiplication table given in Table 3.3. By construction, we have for each of the matrices

$$D^{\mathrm{reg}}(B)_{A_k^{-1},A_j} = \begin{cases} 1 & \text{if} \quad A_k^{-1} A_j = B \\ 0 & \text{otherwise}\,, \end{cases} \tag{3.34}$$

$$D^{\mathrm{reg}}(C)_{A_j^{-1},A_i} = \begin{cases} 1 & \text{if} \quad A_j^{-1} A_i = C \\ 0 & \text{otherwise}\,. \end{cases} \tag{3.35}$$

Therefore in the sum $\sum_{A_j} D^{\rm reg}(B)_{A_k^{-1},A_j} D^{\rm reg}(C)_{A_j^{-1},A_i}$ of (3.33), we have only nonzero entries when

$$BC = (A_k^{-1} \underbrace{A_j)(A_j^{-1}}_{1} A_i) = A_k^{-1} A_i \,. \tag{3.36}$$

But this coincides with the definition of $D^{\rm reg}(BC)$:

$$D^{\rm reg}(BC)_{A_k^{-1},A_i} = \begin{cases} 1 & \text{if} \quad A_k^{-1}A_i = BC \\ 0 & \text{otherwise}\,. \end{cases} \tag{3.37}$$

Therefore $D^{\rm reg}$ is, in fact, a representation of the group $A_1, \ldots, A_h$, completing the proof.

The following theorem allows us to find all the irreducible representations from the regular representation.

Theorem. *The regular representation contains each irreducible representation a number of times equal to the dimensionality of the representation.*

(For the group $P(3)$, this theorem says that $D^{\rm reg}$ contains $D^{(\Gamma_1)}$ once, $D^{(\Gamma_{1'})}$ once, and $D^{(\Gamma_2)}$ twice so that the regular representation of $P(3)$ would be of dimensionality 6.)

Proof. Since $D^{\rm reg}$ is a reducible representation, we can write for the characters (see (3.16))

$$\chi^{\rm reg}(\mathcal{C}_k) = \sum_{\Gamma_i} a_i \chi^{(\Gamma_i)}(\mathcal{C}_k)\,, \tag{3.38}$$

where $\sum_{\Gamma_i}$ is the sum over the irreducible representations and the a_i coefficients have been shown to be unique (3.20) and given by

$$a_i = \frac{1}{h} \sum_k N_k \left[\chi^{(\Gamma_i)}(\mathcal{C}_k)\right]^* \chi^{\rm reg}(\mathcal{C}_k)\,. \tag{3.39}$$

We note that $N_E = 1$ for the identity element, which is in a class by itself. But by construction $\chi^{\rm reg}(\mathcal{C}_k) = 0$ unless $\mathcal{C}_k = E$ in which case $\chi^{\rm reg}(E) = h$. Therefore $a_i = \chi^{(\Gamma_i)}(E) = \ell_i$, where $\chi^{(\Gamma_i)}$ is the trace of an ℓ_i dimensional unit matrix, thereby completing the proof.

The theorem (3.38) that we have just proven tells us that the regular representation contains each irreducible representation of the group at least once. To obtain these irreducible representations explicitly, we have to carry out a similarity transformation which brings the matrices of the regular representation into block diagonal form. It turns out to be very messy to extract the matrices of the regular representation – in fact, it is so tedious to do this operation that it does not even make an instructive homework problem.

It is much easier to write down the matrices which generate the symmetry operations of the group directly.

Consider for example the permutation group of three objects $P(3)$ which is isomorphic to the symmetry operations of a regular triangle (Sect. 1.2). The matrices for D and F generate rotations by $\pm 2\pi/3$ about the z axis, which is $\perp$ to the plane of the triangle. The A matrix represents a rotation by $\pm\pi$ about the y axis while the B and C matrices represent rotations by $\pm\pi$ about axes in the x–y plane which are $\pm 120°$ away from the y axis. In setting up a representation, it is advantageous to write down those matrices which can be easily written down – such as E, A, D, F. The remaining matrices such as B and C can then be found through the multiplication table. □

We will now make use of the regular representation to prove a useful theorem for setting up character tables. This is the most useful application of the regular representation for our purposes.

Theorem. *The order of a group h and the dimensionality ℓ_j of its irreducible representations Γ_j are related by*

$$\sum_j \ell_j^2 = h\,. \tag{3.40}$$

We had previously found (2.70) that $\sum_j \ell_j^2 \leq h$. The regular representation allows us to prove that it is the equality that applies.

Proof. By construction, the regular representation is of dimensionality h which is the number of elements in the group and in the multiplication table. But each irreducible representation of the group is contained ℓ_j times in the regular representation (see (3.38)) so that

$$\chi^{\mathrm{reg}}(E) = h = \sum_{\Gamma_j} \underbrace{a_j}_{\ell_j} \underbrace{\chi^{\Gamma_j}(E)}_{\ell_j} = \sum_{\Gamma_j} {\ell_j}^2\,, \tag{3.41}$$

where one ℓ_j comes from the number of times each irreducible representation is contained in the regular representation and the second ℓ_j is the dimension of the irreducible representation Γ_j.

We thus obtain the result

$$\sum_j \ell_j^2 = h\,, \tag{3.42}$$

where $\sum_j$ is the sum over irreducible representations. For example for $P(3)$, we have $\ell_1 = 1$, $\ell_{1'} = 1$, $\ell_2 = 2$ so that $\sum \ell_j^2 = 6 = h$. □

3.8 Setting up Character Tables

For many applications it is sufficient to know just the character table without the actual matrix representations for a particular group. So far, we have only set up the character table by taking traces of the irreducible representations – i.e., from the definition of χ. For the most simple cases, the character table can be constructed using the results of the theorems we have just proved – without knowing the representations themselves. In practice, the character tables that are needed to solve a given problem are found either in books or in journal articles. The examples in this section are thus designed to show the reader how character tables are constructed, should this be necessary. Our goal is further to give some practice in using the theorems proven in Chap. 3.

A summary of useful rules for the construction of character tables is given next.

(a) The number of irreducible representations is equal to the number of classes (Sect. 3.5). The number of classes is found most conveniently from the classification of the symmetry operations of the group. Another way to find the classes is to compute all possible conjugates for all group elements using the group multiplication table.
(b) The dimensionalities of the irreducible representations are found from $\sum_i \ell_i^2 = h$ (see (3.42)). For simple cases, this relation uniquely determines the dimensionalities of the irreducible representations. For example, the permutation group of three objects $P(3)$ has three classes and therefore three irreducible representations. The identity representation is always present, so that one of these must be one-dimensional (i.e., the matrix for the identity element of the group is the unit matrix). So this gives $1^2+?^2+?^2 = 6$.This equation only has one integer solution, namely $1^2 + 1^2 + 2^2 = 6$. No other solution works!
(c) There is always a whole row of 1s in the character table for the identity representation.
(d) The first column of the character table is always the trace for the unit matrix representing the identity element or class. This character is always ℓ_i, the dimensionality of the $(\ell_i \times \ell_i)$ unit matrix. Therefore, the first column of the character table is also filled in.
(e) For all representations other than the identity representation Γ_1, the following relation is satisfied:

$$\sum_k N_k \chi^{(\Gamma_i)}(\mathcal{C}_k) = 0\,, \tag{3.43}$$

where $\sum_k$ denotes the sum on classes. Equation (3.43) follows from the wonderful orthogonality theorem for character and taking the identity representation Γ_1 as one of the irreducible representations.

If there are only a few classes in the group, (3.43) often uniquely determines the characters for several of the irreducible representations; particularly for the one-dimensional representations.
(f) The Wonderful Orthogonality Theorem for character works on rows of the character table:

$$\sum_k \left[\chi^{(\Gamma_i)}(\mathcal{C}_k)\right]^* \chi^{(\Gamma_j)}(\mathcal{C}_k)N_k = h\delta_{\Gamma_i,\Gamma_j} . \tag{3.44}$$

This theorem can be used both for orthogonality (different rows) or for normalization (same rows) of the characters in an irreducible representation and the complex conjugate can be applied either to the $\chi^{(\Gamma_i)}(\mathcal{C}_k)$ or to the $\chi^{(\Gamma_j)}(\mathcal{C}_k)$ terms in (3.44) since the right hand side of (3.44) is real.

(g) The second orthogonality theorem works for columns of the character table:

$$\sum_{\Gamma_i} \left[\chi^{(\Gamma_i)}(\mathcal{C}_k)\right]^* \chi^{(\Gamma_i)}(\mathcal{C}_{k'}) = \frac{h}{N_k}\delta_{kk'} . \tag{3.45}$$

This relation can be used both for orthogonality (different columns) or normalization (same columns), as the wonderful orthogonality theorem for character.

(h) From the second orthogonality theorem for character, and from the character for the identity class

$$\chi^{(\Gamma_i)}(E) = \ell_i \tag{3.46}$$

we see that the characters for all the other classes obey the relation

$$\sum_{\Gamma_i} \chi^{(\Gamma_i)}(\mathcal{C}_k)\ell_i = 0 , \tag{3.47}$$

where $\sum_{\Gamma_i}$ denotes the sum on irreducible representations and ℓ_i is the dimensionality of representation Γ_i. Equation (3.47) follows from the wonderful orthogonality theorem for character, and it uses the identity representations as one of the irreducible representations, and for the second any but the identity representation ($\Gamma_i \neq \Gamma_1$) can be used.

With all this machinery it is often possible to complete the character tables for simple groups without an explicit determination of the matrices for a representation.

Let us illustrate the use of the rules for setting up character tables with the permutation group of three objects, $P(3)$. We fill in the first row and first column of the character table immediately from rules #3 and #4 in the earlier list (see Table 3.4).

In order to satisfy #5, we know that $\chi^{(\Gamma_{1'})}(\mathcal{C}_2) = -1$ and $\chi^{(\Gamma_{1'})}(\mathcal{C}_3) = 1$, which we add to the character table (Table 3.5).

Table 3.4. Character table for P(3) – Step 1

	$\mathcal{C}_1$	$3\mathcal{C}_2$	$2\mathcal{C}_3$
Γ_1	1	1	1
$\Gamma_{1'}$	1		
Γ_2	2		

Table 3.5. Character table for P(3) – Step 2

	$\mathcal{C}_1$	$3\mathcal{C}_2$	$2\mathcal{C}_3$
Γ_1	1	1	1
$\Gamma_{1'}$	1	-1	1
Γ_2	2		

Table 3.6. Character table for P(3)

	$\mathcal{C}_1$	$3\mathcal{C}_2$	$2\mathcal{C}_3$
Γ_1	1	1	1
$\Gamma_{1'}$	1	-1	1
Γ_2	2	0	-1

Table 3.7. Multiplication table for the cyclic group of three rotations by $2\pi/3$ about a common axis

	E	C_3	C_3^2
E	E	C_3	C_3^2
C_3	C_3	C_3^2	E
C_3^2	C_3^2	E	C_3

Now apply the second orthogonality theorem using columns 1 and 2 and then again with columns 1 and 3, and this completes the character table, thereby obtaining Table 3.6.

Let us give another example of a character table which illustrates another principle that not all entries in a character table need to be real. Such a situation can occur in the case of cyclic groups. Consider a group with three symmetry operations:

- E – identity,
- C_3 – rotation by $2\pi/3$,
- C_3^2 – rotation by $4\pi/3$.

See Table 3.7 for the multiplication table for this group. All three operations in this cyclic group C_3 are in separate classes as can be easily seen by conjugation of the elements. Hence there are three classes and three irreducible representations to write down. The character table we start with is obtained by following Rules #3 and #4 (Table 3.8). Orthogonality of Γ_2 to Γ_1 yields the algebraic relation: $1 + a + b = 0$.

Since $C_3^2 = C_3C_3$ and $C_3^2C_3 = E$, it follows that $b = a^2$ and $ab = a^3 = 1$, so that $a = \exp(2\pi i/3)$. Then, orthogonality of the second column with the first yields $c = \exp(4\pi i/3)$ and orthogonality of the third column with the first column yields $d = [\exp(4\pi i/3)]^2$. From this information we can readily complete the Character Table 3.9, where $\omega = \exp[2\pi i/3]$. Such a group

Table 3.8. Character table for Cyclic Group C_3

	E	C_3	C_3^2
Γ_1	1	1	1
Γ_2	1	a	b
Γ_3	1	c	d

Table 3.9. Character table for cyclic group C_3

	E	C_3	C_3^2
Γ_1	1	1	1
Γ_2	1	ω	ω^2
Γ_3	1	ω^2	ω

often enters into a physical problem which involves time inversion symmetry, where the energy levels corresponding to Γ_2 and Γ_3 are degenerate (see Chap. 16).

This idea of the cyclic group can be applied to a four-element group: E, C_2, C_4, C_4^3 – to a five-element group: E, C_5, C_5^2, C_5^3, C_5^4 – and to a six-element group: E, C_6, C_3, C_2, C_3^2, C_6^5, etc. In each case, use the fact that the Nth roots of unity sum to zero so that each Γ_j is orthogonal to Γ_1 and by the rearrangement theorem each Γ_j is orthogonal to $\Gamma_{j'}$. For the case of Bloch's theorem, we have an N-element group with characters that comprise the Nth roots of unity $\omega = \exp[2\pi i/N]$.

All these cyclic groups are Abelian so that each element is in a class by itself. The representations for these groups correspond to the multiplication tables, which therefore contain the appropriate collections of roots of unity.

The character tables for all the point groups used in this chapter are listed in Appendix A. The notation used in these tables is discussed in more detail in the next sections.

3.9 Schoenflies Symmetry Notation

There are two point group notations that are used for the symmetry operations in the character tables printed in books and journals. One is the Schoenflies symmetry notation, which is described in this section and the other is the Hermann–Mauguin notation that is used by the crystallography community and is summarized in Sect. 3.10. For the Schoenflies system the following notation is commonly used:

- E = Identity
- C_n = rotation through $2\pi/n$. For example C_2 is a rotation of 180°. Likewise C_3 is a rotation of 120°, while C_6^2 represents a rotation of 60° followed

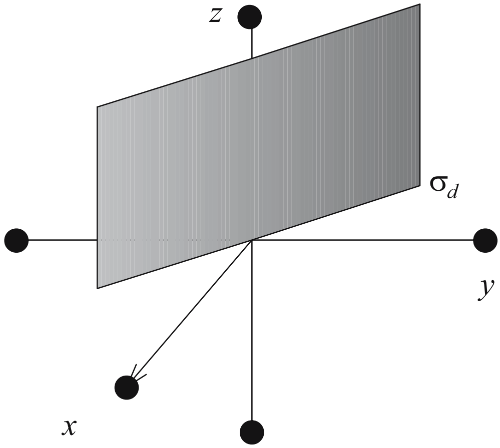

Fig. 3.1. Schematic illustration of a dihedral symmetry axis. The reflection plane containing the diagonal of the square and the fourfold axis is called a dihedral plane. For this geometry $\sigma_d(x, y, z) = (-y, -x, z)$

by another rotation of 60° about the same axis so that $C_6^2 = C_3$. In a Bravais lattice it can be shown that n in C_n can only assume values of $n = 1$, 2, 3, 4, and 6. The observation of a diffraction pattern with fivefold symmetry in 1984 was therefore completely unexpected, and launched the field of quasicrystals, where a six-dimensional space is used for obtaining crystalline periodicity.

- σ = reflection in a plane.
- σ_h = reflection in a "horizontal" plane. The reflection plane here is perpendicular to the axis of highest rotational symmetry.
- σ_v = reflection in a "vertical" plane. The reflection plane here contains the axis of highest rotational symmetry.
- σ_d is the reflection in a diagonal plane. The reflection plane here is a vertical plane which bisects the angle between the twofold axes $\perp$ to the principal symmetry axis. An example of a diagonal plane is shown in Fig. 3.1. σ_d is also called a dihedral plane.
- i is the inversion which takes

$$\begin{cases} x \to -x \\ y \to -y \\ z \to -z\,. \end{cases}$$

- S_n is the improper rotation through $2\pi/n$, which consists of a rotation by $2\pi/n$ followed by a reflection in a horizontal plane. Alternatively, we can define S_n as a rotation by $4\pi/n$ followed by the inversion.
- iC_n = compound rotation–inversion, which consists of a rotation followed by an inversion.

In addition to these point group symmetry operations, there are several space group symmetry operations, such as translations, glide planes, screw axes, etc. which are discussed in Chap. 9. The point groups, in contrast to the space groups, exhibit a point that never moves under the application of all symmetry operations. There are *32 common point groups* for crystallographic systems ($n = 1, 2, 3, 4, 6$), and the character tables for these 32 point groups are given in many standard group theory texts. For convenience we also list the character tables for these point groups in Appendix A (Tables A.1–A.32). Tables A.22–A.28 are for groups with fivefold symmetry axes and such tables are not readily found in group theory books, but have recently become important, because of the discovery of quasicrystals, C_{60}, and related molecules. Note that the tables for fivefold symmetry are: C_5 (Table A.22); C_{5v} (Table A.23); $C_{5h} \equiv C_5 \otimes \sigma_h$; D_5 (Table A.24); D_{5d} (Table A.25); D_{5h} (Table A.26); I (Table A.27); and I_h (Table A.28). Recurrent in these tables is the "golden mean," $\tau = (1 + \sqrt{5})/2$ where $\tau - 1 = 2\cos(2\pi/5) = 2\cos 72°$. These are followed by Tables A.33 and A.34 for the semi-infinite groups $C_{\infty v}$ and $D_{\infty h}$, discussed later in this section.

Certain patterns can be found between the various point groups. Groups $C_1, C_2, \ldots, C_6$ only have n-fold rotations about a simple symmetry axis C_n (see for example Table A.15) and are cyclic groups, mentioned in Sect. 3.8. Groups C_{nv} have, in addition to the n-fold axes, vertical reflection planes σ_v (e.g., Table A.16). Groups C_{nh} have, in addition to the n-fold axes, horizontal reflection planes σ_h and include each operation C_n together with the compound operations C_n followed by σ_h (Tables A.3 and A.11 illustrate this relation between groups). The groups S_2, S_4, and S_6 have mostly compound operations (see Tables A.2, A.17, and A.20). The groups denoted by D_n are dihedral groups and have non-equivalent symmetry axes in perpendicular planes (e.g., Table A.18). The group of the operations of a square is D_4 and has in addition to the principal fourfold axes, two sets of non-equivalent twofold axes (Table A.18). We use the notation C_2' to indicate that these twofold axis are in a different plane (see also Table A.12 for group D_3, where this same situation occurs). When non-equivalent axes are combined with mirror planes we get groups like D_{2h}, D_{3h}, etc. (see Tables A.8 and A.14). There are five cubic groups T, O, T_d, T_h, and O_h. These groups have no principal axis but instead have four threefold axes (see Tables A.29–A.32).

3.10 The Hermann–Mauguin Symmetry Notation

There is also a second notation for symmetry operations and groups, namely the *Hermann–Mauguin or international notation*, which is used in the International Tables for X-Ray Crystallography, a standard structural and symmetry reference book. The international notation is what is usually found in crystallography textbooks and various materials science journals. For that reason

Table 3.10. Comparison between Schoenflies and Hermann–Mauguin notation

	Schoenflies	Hermann–Mauguin
rotation	C_n	n
rotation–inversion	iC_n	$\bar{n}$
mirror plane	σ	m
horizontal reflection plane $\perp$ to n-fold axes	σ_h	n/m
n-fold axes in vertical reflection plane	σ_v	nm
two non-equivalent vertical reflection planes	$\sigma_{v'}$	nmm

Table 3.11. Comparison of notation for proper and improper rotations in the Schoenflies and International systems

proper rotations		improper rotations	
international	Schoenflies	international	Schoenflies
1	C_1	$\bar{1}$	S_2
2	C_2	$\bar{2} \equiv m$	σ
3	C_3	$\bar{3}$	S_6^{-1}
3_2	C_3^{-1}	$\bar{3}_2$	S_6
4	C_4	$\bar{4}$	S_4^{-1}
4_3	C_4^{-1}	$\bar{4}_3$	S_4
5	C_5	$\bar{5}$	S_{10}
5_4	C_5^{-1}	$\bar{5}_4$	S_{10}^{-1}
6	C_6	$\bar{6}$	S_3^{-1}
6_5	C_6^{-1}	$\bar{6}_5$	S_3

it is also necessary to become familiar with this notation. The general correspondence between the two notations is shown in Table 3.10 for rotations and mirror planes. The Hermann–Mauguin notation $\bar{n}$ means iC_n which is equivalent to a rotation of $2\pi/n$ followed by or preceded by an inversion. A string of numbers like 422 (see Table A.18) means that there is a fourfold major symmetry axis (C_4 axis), and perpendicular to this axis are two inequivalent sets of twofold axes C_2' and C_2'', such as occur in the group of the square (D_4). If there are several inequivalent horizontal mirror planes like

$$\frac{2}{m}, \quad \frac{2}{m}, \quad \frac{2}{m},$$

an abbreviated notation mmm is sometimes used [see notation for the group D_{2h} (Table A.8)]. The notation $4mm$ (see Table A.16) denotes a fourfold axis and two sets of vertical mirror planes, one set through the axes C_4 and denoted by $2\sigma_v$ and the other set through the bisectors of the $2\sigma_v$ planes and denoted by the dihedral vertical mirror planes $2\sigma_{\mathrm{d}}$. Table 3.11 is useful in relating the two kinds of notations for rotations and improper rotations.

3.11 Symmetry Relations and Point Group Classifications

In this section we summarize some useful relations between symmetry operations and give the classification of point groups. Some useful relations on the commutativity of symmetry operations are:

(a) Inversion commutes with all point symmetry operations.
(b) All rotations about the same axis commute.
(c) All rotations about an arbitrary rotation axis commute with reflections across a plane perpendicular to this rotation axis.
(d) Two twofold rotations about perpendicular axes commute.
(e) Two reflections in perpendicular planes will commute.
(f) Any two of the symmetry elements σ_h, S_n, C_n (n = even) implies the third.

If we have a major symmetry axis $C_n (n \geq 2)$ and there are either twofold axes C_2 or vertical mirror planes σ_v, then there will generally be more than one C_2 or σ_v symmetry operations. In some cases these symmetry operations are in the same class and in the other cases they are not, and this distinction can be made by use of conjugation (see Sect. 1.6).

The classification of the 32 crystallographic point symmetry groups shown in Table 3.12 is often useful in making practical applications of character tables in textbooks and journal articles to specific materials.

In Table 3.12 the first symbol in the Hermann–Mauguin notation denotes the principal axis or plane. The second symbol denotes an axis (or plane) perpendicular to this axis, except for the cubic groups, where the second symbol refers to a $\langle 111 \rangle$ axis. The third symbol denotes an axis or plane that is $\perp$ to the first axis and at an angle of π/n with respect to the second axis.

In addition to the 32 crystallographic point groups that are involved with the formation of three-dimensional crystals, there are nine symmetry groups that form clusters and molecules which show icosahedral symmetry or are related to the icosahedral group I_h. We are interested in these species because they can become part of crystallographic structures. Examples of such clusters and molecules are fullerenes. The fullerene C_{60} has full icosahedral symmetry I_h (Table A.28), while C_{70} has D_{5h} symmetry (Table A.26) and C_{80} has D_{5d} symmetry (Table A.25). The nine point groups related to icosahedral symmetry that are used in solid state physics, as noted earlier, are also listed in Table 3.12 later that double line.

Table 3.12. The extended 32 crystallographic point groups and their symbols[a]

system	Schoenflies symbol	Hermann–Mauguin symbol[b] full	abbreviated	examples
triclinic	C_1	1	1	
	$C_i, (S_2)$	$\bar{1}$	$\bar{1}$	Al_2SiO_5
monoclinic	$C_{1h}, (S_1)$	m	m	KNO_2
	C_2	2	2	
	C_{2h}	$2/m$	$2/m$	
orthorhombic	C_{2v}	$2mm$	mm	
	$D_2, (V)$	222	222	
	$D_{2h}, (V_h)$	$2/m\ 2/m\ 2/m$	mmm	I, Ga
tetragonal	C_4	4	4	
	S_4	$\bar{4}$	$\bar{4}$	
	C_{4h}	$4/m$	$4/m$	$CaWO_4$
	$D_{2d}, (V_d)$	$\bar{4}2m$	$\bar{4}2m$	
	C_{4v}	$4mm$	$4mm$	
	D_4	422	42	
	D_{4h}	$4/m\ 2/m\ 2/m$	$4/mmm$	TiO_2, In, β-Sn
rhombohedral	C_3	3	3	AsI_3
	$C_{3i}, (S_6)$	$\bar{3}$	$\bar{3}$	$FeTiO_3$
	C_{3v}	$3m$	$3m$	
	D_3	32	32	Se
	D_{3d}	$\bar{3}2/m$	$\bar{3}m$	Bi, As, Sb, Al_2O_3
hexagonal	$C_{3h}, (S_3)$	$\bar{6}$	$\bar{6}$	
	C_6	6	6	
	C_{6h}	$6/m$	$6/m$	
	D_{3h}	$\bar{6}2m$	$\bar{6}2m$	
	C_{6v}	$6mm$	$6mm$	ZnO, NiAs
	D_6	622	62	CeF_3
	D_{6h}	$6/m\ 2/m\ 2/m$	$6/mmm$	Mg, Zn, graphite

Footnote (a): The usual 32 crystallographic point groups are here extended by including 9 groups with 5 fold symmetry and are identified here as icosahedral point groups.

Footnote (b): In the Hermann–Mauguin notation, the symmetry axes parallel to and the symmetry planes perpendicular to each of the "principal" directions in the crystal are named in order. When there is both an axis parallel to and a plane normal to a given direction, these are indicated as a fraction; thus $6/m$ means a sixfold rotation axis standing perpendicular to a plane of symmetry, while $\bar{4}$ denotes a fourfold rotary inversion axis. In some classifications, the rhombohedral (trigonal) groups are listed with the hexagonal groups. Also show are the corresponding entries for the icosahedral groups (see text).

Table 3.12. (continued)

the extended 32 crystallographic point groups and their symmetries				
system	Schoenflies symbol	Hermann–Mauguin symbol full	abbreviated	examples
cubic	T	23	23	$NaClO_3$
	T_h	$2/m\bar{3}$	$m3$	FeS_2
	T_d	$\bar{4}3m$	$\bar{4}3m$	ZnS
	O	432	43	β-Mn
	O_h	$4/m\ \bar{3}\ 2/m$	$m3m$	NaCl, diamond, Cu
icosahedral	C_5	5	5	
	$C_{5i}, (S_{10})$	$\bar{10}$	$\bar{10}$	
	C_{5v}	$5m$	$5m$	
	C_{5h}, S_5	$\bar{5}$	$\bar{5}$	
	D_5	52	52	
	D_{5d}	$\bar{5}2/m$	$\bar{5}/m$	C_{80}
	D_{5h}	$\bar{10}2m$	$\bar{10}2m$	C_{70}
	I	532	532	
	I_h			C_{60}

It is also convenient to picture many of the point group symmetries with stereograms (see Fig. 3.2). The stereogram is a mapping of a general point on a sphere onto a plane going through the center of the sphere. If the point on the sphere is above the plane it is indicated as a +, and if below as a $\circ$. In general, the polar axis of the stereogram coincides with the principal axis of symmetry. The first five columns of Fig. 3.2 pertain to the crystallographic point group symmetries and the sixth column is for fivefold symmetry.

The five first stereograms on the first row pertaining to groups with a single axis of rotation show the effect of two-, three-, four-, and sixfold rotation axes on a point +. These groups are cyclic groups with only n-fold axes. Note the symmetry of the central point for each group. On the second row we have added vertical mirror planes which are indicated by the solid lines. Since the "vertical" and "horizontal" planes are not distinguishable for C_1, the addition of a mirror plane to C_1 is given in the third row, showing the groups which result from the first row upon addition of horizontal planes. The symbols $\oplus$ indicate the coincidence of the projection of points above and below the plane, characteristic of horizontal mirror planes.

If instead of proper rotations as in the first row, we can also have improper rotations, then the groups on row 4 are generated. Since S_1 is identical with C_{1h}, it is not shown separately; this also applies to $S_3 = C_{3h}$ and to $S_5 = C_{5h}$ (neither of which are shown). It is of interest to note that S_2 and S_6 have inversion symmetry but S_4 does not.

The addition of twofold axes $\perp$ to the principal symmetry axis for the groups in the first row yields the stereograms of the fifth row where the twofold

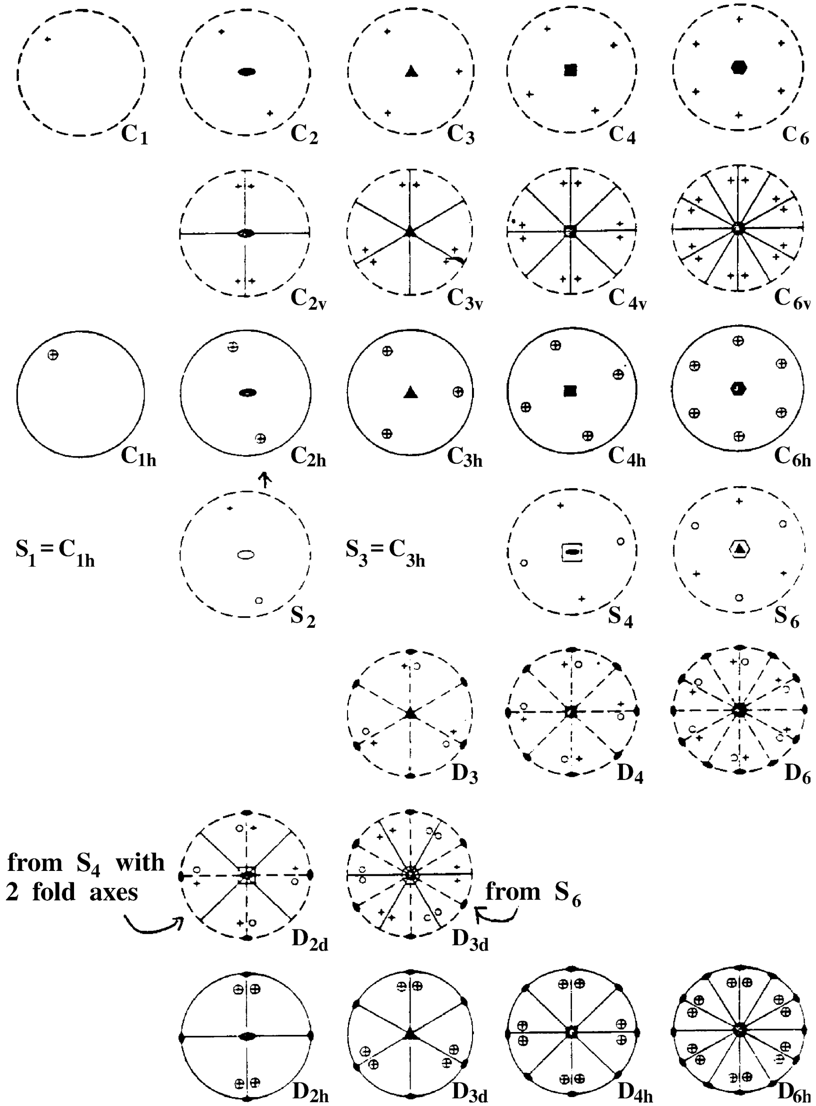

Fig. 3.2. The *first five columns* show stereographic projections of simple crystallographic point groups

axes appear as dashed lines. Here we see that the higher the symmetry of the principal symmetry axis, the greater the number of twofold axes D_5 (not shown) that would have 5 axes separated by 72°.

The addition of twofold axes to the groups on the fourth row yields the stereograms of the sixth row, where D_{2d} comes from S_4, while D_{3d} comes from S_6. Also group D_{5d} (not shown) comes from S_{10}. The addition of twofold axes

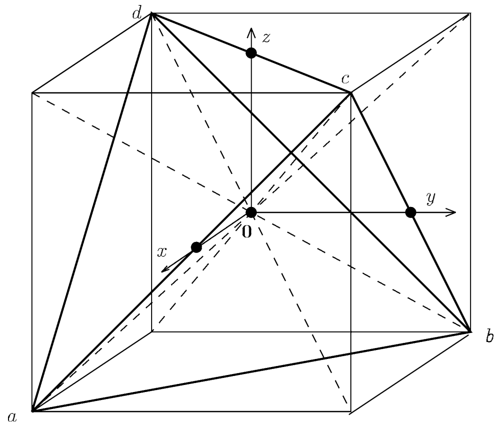

Fig. 3.3. Schematic diagram for the symmetry operations of the group T_d

to S_2 results in C_{2h}. The stereograms on the last row are obtained by adding twofold axes $\perp$ to C_n to the stereograms for the C_{nh} groups on the third row. D_{5h} (not shown) would fall into this category. The effect of adding a twofold axis to C_{1h} is to produce C_{2v}.

The five point symmetry groups associated with cubic symmetry (T, O, T_d, T_h and O_h) are not shown in Fig. 3.2. These groups have higher symmetry and have no single principal axis. The resulting stereograms are very complicated and for this reason are not given in Fig. 3.2. For the same reason the stereograph for the I and I_h icosahedral groups are not given. We give some of the symmetry elements for these groups next.

The group T (or 23 using the International notation) has 12 symmetry elements which include:

1	identity	
3	twofold axes	(x, y, z)
4	threefold axes	(body diagonals – positive rotation)
4	threefold axes	(body diagonals – negative rotations)
12	symmetry elements	

The point group T_h (denoted by $m3$ in the abbreviated International notation or by $2/m3$ in the full International notation) contains all the symmetry operations of T and inversion as well, and is written as $T_h \equiv T \otimes i$, indicating the direct product of the group T and the group C_i having two symmetry elements E, i (see Chap. 6). This is equivalent to adding a horizontal plane of symmetry, hence the notation $2/m$; the symbol 3 means a threefold axis (see Table 3.11). Thus T_h has 24 symmetry elements.

The point group T_d ($\bar{4}3m$) contains the symmetry operations of the regular tetrahedron (see Fig. 3.3), which correspond to the point symmetry for diamond and the zincblende (III–V and II–VI) structures. We list next the 24 symmetry operations of T_d:

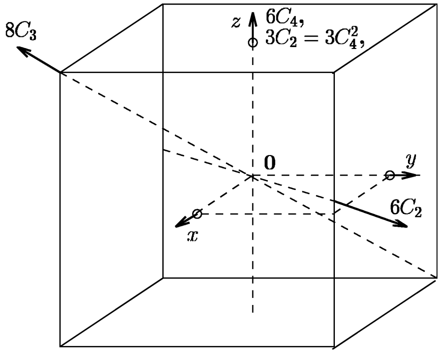

Fig. 3.4. Schematic for the symmetry operations of the group O

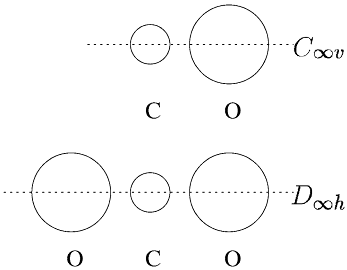

Fig. 3.5. Schematic diagram of the CO molecule with symmetry $C_{\infty v}$ and symmetry operations E, $2C_\phi$, σ_v, and the linear CO_2 molecule in which the inversion operation together with $(E, 2C_\phi, \sigma_v)$ are also present to give the group $D_{\infty h}$

- identity,
- eight C_3 about body diagonals corresponding to rotations of $\pm 2\pi/3$,
- three C_2 about x, y, z directions,
- six S_4 about x, y, z corresponding to rotations of $\pm\pi/2$,
- six σ_d planes that are diagonal reflection planes.

The cubic groups are O (432) and O_h ($m3m$), and they are shown schematically in Fig. 3.4.

The operations for group O as shown in Fig. 3.4 are E, $8C_3$, $3C_2 = 3C_4^2$, $6C_2$, and $6C_4$. To get O_h we combine these 24 operations with inversion to give 48 operations in all. We note that the second symbol in the Hermann–Mauguin (International) notation for all five cubic groups is for the $\langle 111 \rangle$ axes rather than for an axis $\perp$ to the principal symmetry axis.

In addition to the 32 crystallographic point groups and to the eight fivefold point groups, the character tables contain listings for $C_{\infty v}$ (Table A.33) and $D_{\infty h}$ (Table A.34) which have full rotational symmetry around a single axis, and therefore have an ∞ number of symmetry operations and classes. These two groups are sometimes called the semi-infinite groups because they have an infinite number of operations about the major symmetry axis. An example of $C_{\infty v}$ symmetry is the CO molecule shown in Fig. 3.5.

Here the symmetry operations are E, $2C_\phi$, and σ_v. The notation C_ϕ denotes an axis of full rotational symmetry and σ_v denotes the corresponding infinite array of vertical planes. The group $D_{\infty h}$ has in addition the inversion operation which is compounded with each of the operations in $C_{\infty v}$, and this is written as $D_{\infty h} = C_{\infty v} \otimes i$ (see Chap. 6). An example of a molecule with $D_{\infty h}$ symmetry is the CO_2 molecule (see Fig. 3.5).

Selected Problems

3.1. (a) Explain the symmetry operations pertaining to each class of the point group D_{3h}. You may find the stereograms on p. 51 useful.

(b) Prove that the following irreducible representations E_1 and E_2 in the group D_5 (see Table A.24) are orthonormal.

(c) Given the group T (see Table A.29), verify that the equality

$$\sum_j \ell_j^2 = h$$

is satisfied. What is the meaning of the two sets of characters given for the two-dimensional irreducible representation E? Are they orthogonal to each other or are they part of the same irreducible representation?

(d) Which symmetry operation results from multiplying the operations σ_v and σ_d in group C_{4v}? Can you obtain this information from the character table? If so, how?

3.2. Consider an A_3B_3 molecule consisting of $3A$ atoms at the corners of a regular triangle and $3B$ atoms at the corners of another regular triangle, rotated by 60° with respect to the first.

(a) Consider the A and B atoms alternately occupy the corners of a planar regular hexagon. What are the symmetry operations of the symmetry group and what is the corresponding point group? Make a sketch of the atomic equilibrium positions for this case.

(b) If now the A atoms are on one plane and the B atoms are on another parallel plane, what are the symmetry operations and point group?

(c) If now all atoms in (a) are of the same species, what then are the symmetry operations of the appropriate point group, and what is this group?

(d) Which of these groups are subgroups of the highest symmetry group? How could you design an experiment to test your symmetry group identifications?

3.3. (a) What are the symmetry operations of a regular hexagon?

(b) Find the classes. Why are not all the two-fold axes in the same class?

(c) Find the self-conjugate subgroups, if any.
(d) Identify the appropriate character table.
(e) For some representative cases (two cases are sufficient), check the validity of the "Wonderful Orthogonality and Second Orthogonality Theorems" on character, using the character table in (d).

3.4. Suppose that you have the following set of characters: $\chi(E) = 4$, $\chi(\sigma_h) = 2$, $\chi(C_3) = 1$, $\chi(S_3) = -1$, $\chi(C_2') = 0$, $\chi(\sigma_v) = 0$.

(a) Do these characters correspond to a representation of the point group D_{3h}? Is it irreducible?
(b) If the representation is reducible, find the irreducible representations contained therein.
(c) Give an example of a molecule with D_{3h} symmetry.

3.5. Consider a cube that has O_h symmetry.

(a) Which symmetry group is obtained by squeezing the cube along one of the main diagonals?
(b) Which symmetry group is obtained if you add mirror planes perpendicular to the main diagonals, and have a mirror plane crossing these main diagonals in the middle.