

Chapter 2

The Crystallographic Groups

2.1 The Orthogonal Group in Three-Space

Let R_3 be three-dimensional real Euclidean space. We erect a cartesian coordinate system with origin C in this space and associate with each point P in R_3 a unique triple of real numbers (x_1, x_2, x_3) , the projections of P on the three mutually perpendicular coordinate axes. It is useful to think of R_3 as a three-dimensional vector space with elements $\mathbf{x} = (x_1, x_2, x_3) = \sum_{i=1}^3 x_i \mathbf{e}_i$, where $\mathbf{e}_1, \mathbf{e}_2$, and \mathbf{e}_3 are unit vectors along the coordinate axes. As is well known, the bilinear form

$$(1.1) \quad \langle \mathbf{x}, \mathbf{y} \rangle = \sum_{i=1}^3 x_i y_i, \quad \mathbf{x}, \mathbf{y} \in R_3$$

defines an inner product on this space. The norm $\|\mathbf{x}\| = \langle \mathbf{x}, \mathbf{x} \rangle^{1/2}$ is the Euclidean length of the vector \mathbf{x} and

$$(1.2) \quad \cos \varphi = \langle \mathbf{x}, \mathbf{y} \rangle / \|\mathbf{x}\| \|\mathbf{y}\|$$

is the cosine of the angle φ between the vectors \mathbf{x} and \mathbf{y} .

We look for all linear transformations $\mathbf{O}: R_3 \rightarrow R_3$ which preserve length, i.e., all linear transformations \mathbf{O} such that $\langle \mathbf{O}\mathbf{x}, \mathbf{O}\mathbf{x} \rangle = \langle \mathbf{x}, \mathbf{x} \rangle$ for all $\mathbf{x} \in R_3$. Because of the identity

$$(1.3) \quad 4\langle \mathbf{x}, \mathbf{y} \rangle = \langle \mathbf{x} + \mathbf{y}, \mathbf{x} + \mathbf{y} \rangle - \langle \mathbf{x} - \mathbf{y}, \mathbf{x} - \mathbf{y} \rangle$$

it follows that

$$(1.4) \quad \langle \mathbf{O}\mathbf{x}, \mathbf{O}\mathbf{y} \rangle = \langle \mathbf{x}, \mathbf{y} \rangle$$

and the transformation \mathbf{O} also preserves angle. That is, the angle between the vectors \mathbf{x} and \mathbf{y} is equal to the angle between vectors \mathbf{Ox} and \mathbf{Oy} .

To compute the possible length-preserving transformations \mathbf{O} we pass to matrices. Recall that the matrix T of a linear transformation $\mathbf{T}: \mathbb{R}_3 \rightarrow \mathbb{R}_3$ with respect to the basis $\mathbf{e}_1, \mathbf{e}_2, \mathbf{e}_3$ is defined by $T = (T_{ij})$, $1 \leq i, j \leq 3$, where

$$(1.5) \quad \mathbf{Te}_j = \sum_{i=1}^3 T_{ij} \mathbf{e}_i.$$

The identity operator $\mathbf{Ex} = \mathbf{x}$ has the matrix $E_3 = (\delta_{ij})$, where δ_{ij} is the Kronecker delta. The product \mathbf{TQ} of two transformations defined by $\mathbf{TQx} = \mathbf{T}(\mathbf{Qx})$ corresponds to the matrix product TQ where $(TQ)_{ij} = \sum_k T_{ik} Q_{kj}$. Furthermore, the inverse \mathbf{T}^{-1} of an invertible operator \mathbf{T} corresponds to the inverse matrix T^{-1} of the nonsingular matrix T .

Using the fact that $\mathbf{Ox} = \sum_{i,j} O_{ij} x_j \mathbf{e}_i$ and writing the equation $\langle \mathbf{Ox}, \mathbf{Oy} \rangle = \langle \mathbf{x}, \mathbf{y} \rangle$ in component form, we obtain the result

$$(1.6) \quad \sum_{i=1}^3 O_{ij} O_{ik} = \delta_{jk}$$

or $O^t O = E_3$ in terms of matrix multiplication. Here, O^t is the transpose of the matrix O , $O_{ij}^t = O_{ji}$. Thus $O^t = O^{-1}$ is a necessary and sufficient condition that the operators \mathbf{O} preserve inner product. Let $O(3) = \{3 \times 3 \text{ matrices } O: O^t O = E_3\}$. Clearly the matrices in $O(3)$ are all nonsingular. Now, $(O_1 O_2)^t (O_1 O_2) = O_2^t O_1^t O_1 O_2 = O_2^t O_2 = E_3$ if $O_1, O_2 \in O(3)$, so $O_1 O_2 \in O(3)$. Furthermore, $E_3 \in O(3)$ and $(O_1^{-1})^t O_1^{-1} = O_1 O_1^{-1} = E_3$, so $O_1^{-1} \in O(3)$. Thus, $O(3)$ is a group, the **real orthogonal group** in three-space. The operators \mathbf{O} also form a group and the correspondence $\mathbf{O} \leftrightarrow O$ defines an isomorphism between the two groups. Both groups are usually called $O(3)$. Any abstract group-theoretic property which holds for one realization of $O(3)$ automatically holds for the other. We shall sometimes use the operator form of the group and at other times use the matrix form.

Lemma 2.1. $\det O = \pm 1$ if $O \in O(3)$.

Proof. Since $O^t O = E_3$ it follows that $\det(O^t O) = 1$. But, $\det(O^t O) = (\det O^t) \cdot (\det O) = (\det O)^2$.

Both signs of the determinant occur. Indeed, E_3 and $I_3 = -E_3$ are elements of $O(3)$ with $\det E_3 = 1$ and $\det I_3 = -1$. The operator \mathbf{I} with matrix I_3 is defined by $\mathbf{Ix} = -\mathbf{x}$, all $\mathbf{x} \in \mathbb{R}_3$, and called the **inversion** operator. Note that $\mathbf{I}^2 = \mathbf{E}$. Since $\det(O_1 O_2) = (\det O_1) \cdot (\det O_2)$ it follows that the set

$$(1.7) \quad SO(3) = \{O \in O(3): \det O = +1\}$$

forms a subgroup of $O(3)$, called the **special orthogonal group (proper orthogonal group) in three-space** or just the **rotation group**. The map $O \rightarrow \det O$ defines a homomorphism of $O(3)$ onto the cyclic group of order two with elements $1 = e$ and -1 . The kernel of this homomorphism is $SO(3)$, which implies that $SO(3)$ is a normal subgroup of $O(3)$. Furthermore, by Theorem 1.5 there are exactly two $SO(3)$ -cosets in $O(3)$: $SO(3)$ and $I_3 \cdot SO(3)$. The elements of the first coset are all proper orthogonal (rotation) matrices and the elements of the second coset are all **improper**, i.e., they have negative determinants. Thus, every improper element O' can be written uniquely in the form $O' = I_3 O$, a rotation followed by inversion.

The groups $O(3)$ and $SO(3)$ have now been realized as transformation groups on the set R_3 . We will show that the elements of $SO(3)$ are exactly the possible geometrical rotations about all axes in R_3 passing through the origin, while $O(3)$ consists of all possible geometrical rotations and rotation-inversions in R_3 that fix the origin.

Theorem 2.1. Let $O \in SO(3)$. Then there is a vector $\mathbf{f}_3 \in R_3$, $\|\mathbf{f}_3\| = 1$, such that $O\mathbf{f}_3 = \mathbf{f}_3$. If $\mathbf{O} \neq \mathbf{E}$ the axis designated by $\pm\mathbf{f}_3$ is called the **axis of rotation**.

Proof. The theorem asserts that the operator \mathbf{O} has a unit eigenvector \mathbf{f}_3 with eigenvalue $\lambda = 1$. This is equivalent to the assertion that $\lambda = 1$ is a solution of the characteristic equation $\det(O - \lambda E_3) = 0$. But $\det(O - E_3) = \det(O^t - E_3^t) = \det(O^{-1} - E_3) = (\det O^{-1}) \cdot [\det(-E_3)] \cdot \det(O - E_3) = -\det(O - E_3)$. Therefore, $\det(O - E_3) = 0$ and $\lambda = 1$ is an eigenvalue of \mathbf{O} . Thus, a desired vector \mathbf{f}_3 exists, though it is not unique.

Now choose unit vectors \mathbf{f}_1 and \mathbf{f}_2 so that $\{\mathbf{f}_1, \mathbf{f}_2, \mathbf{f}_3\}$ is an orthonormal basis for R_3 , i.e., $\langle \mathbf{f}_j, \mathbf{f}_k \rangle = \delta_{jk}$. We will compute the matrix \tilde{O} of \mathbf{O} with respect to this basis. The relations $\langle \mathbf{O}\mathbf{f}_j, \mathbf{O}\mathbf{f}_k \rangle = \langle \mathbf{f}_j, \mathbf{f}_k \rangle = \delta_{jk}$ lead to

$$(1.8) \quad \begin{aligned} \mathbf{O}\mathbf{f}_1 &= \alpha_1 \mathbf{f}_1 + \beta_1 \mathbf{f}_2, & \alpha_1 \alpha_2 + \beta_1 \beta_2 &= 0 \\ \mathbf{O}\mathbf{f}_2 &= \alpha_2 \mathbf{f}_1 + \beta_2 \mathbf{f}_2, & \alpha_1^2 + \beta_1^2 &= 1 \\ \mathbf{O}\mathbf{f}_3 &= \mathbf{f}_3, & \alpha_2^2 + \beta_2^2 &= 1. \end{aligned}$$

These equations have the unique solution ($\det \tilde{O} = 1$)

$$(1.9) \quad \alpha_1 = \beta_2 = \cos \theta, \quad \beta_1 = -\alpha_2 = \sin \theta, \quad 0 \leq \theta < 2\pi,$$

so that the matrix of \mathbf{O} in the \mathbf{f} -basis is

$$(1.10) \quad \tilde{O} = \begin{pmatrix} \cos \theta & -\sin \theta & 0 \\ \sin \theta & \cos \theta & 0 \\ 0 & 0 & 1 \end{pmatrix}.$$

It follows from (1.10) and elementary analytic geometry that \mathbf{O} can be interpreted as a counterclockwise rotation through the angle θ about the axis of rotation \mathbf{f}_3 . We adopt the notation $O = C_{\mathbf{k}}(\theta)$, where $\mathbf{k} = \mathbf{f}_3$ is the axis of rotation and θ is the rotation angle. Note that

$$(1.11) \quad C_{\mathbf{k}}(\theta + \varphi) = C_{\mathbf{k}}(\theta)C_{\mathbf{k}}(\varphi),$$

where we assume $C_{\mathbf{k}}(\alpha + 2\pi) = C_{\mathbf{k}}(\alpha)$. Furthermore, both \mathbf{k} and $-\mathbf{k}$ serve to define the same axis of rotation so

$$(1.12) \quad C_{\mathbf{k}}(\theta) = C_{-\mathbf{k}}(2\pi - \theta).$$

Since O and \tilde{O} are matrices of the same transformation \mathbf{O} viewed in different basis systems, these matrices must be similar, i.e., $\tilde{O} = QOQ^{-1}$, where Q is the orthogonal matrix denoting the change of basis. Thus, O and \tilde{O} have the same determinant and trace. In particular,

$$(1.13) \quad \text{tr } O = \sum_{i=1}^3 O_{ii} = \text{tr } \tilde{O} = 1 + 2 \cos \theta.$$

The improper rotations also have a simple geometrical interpretation. An improper rotation O' can be written uniquely in the form

$$(1.14) \quad O' = I_3 C_{\mathbf{k}}(\pi + \theta) = I_3 C_{\mathbf{k}}(\pi) C_{\mathbf{k}}(\theta) = \sigma_{\mathbf{k}} C_{\mathbf{k}}(\theta),$$

where $\sigma_{\mathbf{k}} = I_3 C_{\mathbf{k}}(\pi)$ is the reflection in the plane through the origin of R_3 , perpendicular to \mathbf{k} . Thus, any improper rotation (rotation-inversion) is equal to a rotation about some axis \mathbf{k} followed by a reflection in the plane perpendicular to \mathbf{k} . We write $S_{\mathbf{k}}(\theta) = \sigma_{\mathbf{k}} C_{\mathbf{k}}(\theta)$.

The conjugacy classes in $O(3)$ and $SO(3)$ have a simple physical significance. The relation

$$(1.15) \quad OC_{\mathbf{k}}(\theta)O^{-1} = C_{\mathbf{Ok}}(\theta), \quad O \in SO(3)$$

shows that all rotations through the angle θ about any axis lie in the same conjugacy class of $SO(3)$. Thus the conjugacy classes can be labeled by the rotation angle θ , $0 \leq \theta \leq \pi$. To prove (1.15) we chose an orthonormal basis $\{\mathbf{f}_j\}$ for R_3 corresponding to $C_{\mathbf{k}}(\theta)$, just as in (1.8). In particular, $\mathbf{f}_3 = \mathbf{k}$. Then $\{\mathbf{Of}_1, \mathbf{Of}_2, \mathbf{Of}_3\}$ is also an orthonormal basis and the matrix of $OC_{\mathbf{k}}(\theta)O^{-1}$ in this new basis is just (1.10) again. Thus $OC_{\mathbf{k}}(\theta)O^{-1}$ is a rotation of angle θ about the axis \mathbf{Ok} .

It is left to the reader to verify the following:

$$(1.16) \quad OC_{\mathbf{k}}(\theta)O^{-1} = C_{\epsilon \mathbf{Ok}}(\theta), \quad OS_{\mathbf{k}}(\theta)O^{-1} = S_{\epsilon \mathbf{Ok}}(\theta), \quad O \in O(3),$$

where $\epsilon = \det O$, which show that the conjugacy classes of $O(3)$ fall into two types. One type consists of all rotations through a fixed angle θ , $0 \leq \theta \leq \pi$, and the other consists of all rotation-inversions through a fixed angle θ' , $0 \leq \theta' \leq \pi$.

2.2 The Euclidean Group

We now seek all transformations \mathbf{T} of R_3 onto R_3 that preserve the distance between any pair of points, i.e.,

$$(2.1) \quad \|\mathbf{T}\mathbf{x} - \mathbf{T}\mathbf{y}\| = \|\mathbf{x} - \mathbf{y}\|, \quad \mathbf{x}, \mathbf{y} \in R_3.$$

Such transformations are called *isometries*. We do not assume that the transformations \mathbf{T} are linear. It may be helpful to think of \mathbf{T} as a permutation of the elements of R_3 which also preserves distance. Let $E(3)$ be the set of all isometries.

Theorem 2.2. $E(3)$ is a group, the Euclidean group in three-space.

Proof. The identity mapping \mathbf{E} is clearly in $E(3)$. If $\mathbf{T} \in E(3)$ and $\mathbf{T}\mathbf{x} = \mathbf{T}\mathbf{y}$ then by (2.1), $\|\mathbf{x} - \mathbf{y}\| = 0$ or $\mathbf{x} = \mathbf{y}$. Therefore, \mathbf{T} is invertible. Corresponding to any two vectors \mathbf{w}, \mathbf{z} in R_3 , there exist unique vectors \mathbf{x}, \mathbf{y} such that $\mathbf{T}\mathbf{x} = \mathbf{w}$ and $\mathbf{T}\mathbf{y} = \mathbf{z}$. Thus $\|\mathbf{T}^{-1}\mathbf{w} - \mathbf{T}^{-1}\mathbf{z}\| = \|\mathbf{x} - \mathbf{y}\| = \|\mathbf{T}\mathbf{x} - \mathbf{T}\mathbf{y}\| = \|\mathbf{w} - \mathbf{z}\|$, where we have made use of (2.1) again, and $\mathbf{T}^{-1} \in E(3)$. It is an elementary argument to show that the product $\mathbf{T}_1\mathbf{T}_2\mathbf{x} = \mathbf{T}_1(\mathbf{T}_2\mathbf{x})$ of $\mathbf{T}_1, \mathbf{T}_2 \in E(3)$ is again in $E(3)$. Q.E.D.

As its name suggests, the Euclidean group is basic to the study of Euclidean geometry. In Euclidean geometry, two subsets S, S' of R_3 are said to be **congruent** if there is a $\mathbf{T} \in E(3)$ such that $S' = \mathbf{T}S$, i.e., if the points of S can be made coincident with the points of S' by a distance-preserving transformation. Since congruent triangles have corresponding angles equal, it is easy to show that each $\mathbf{T} \in E(3)$ also preserves the angle between intersecting straight lines.

Among the elements of $E(3)$ the easiest to construct are the **translations** $\mathbf{T}_a, \mathbf{a} \in R_3$:

$$(2.2) \quad \mathbf{T}_a\mathbf{x} = \mathbf{x} + \mathbf{a}, \quad \mathbf{x} \in R_3.$$

Under \mathbf{T}_a each point of R_3 is displaced by \mathbf{a} . The set $T(3)$ of all translations of three-space forms a subgroup of $E(3)$. This subgroup is abelian since

$$(2.3) \quad \mathbf{T}_a\mathbf{T}_b = \mathbf{T}_b\mathbf{T}_a = \mathbf{T}_{(\mathbf{a}+\mathbf{b})}.$$

Let \mathbf{T} be an arbitrary element of $E(3)$ and suppose $\mathbf{T}\mathbf{0} = \mathbf{a}$, where $\mathbf{0} = (0, 0, 0)$ is the origin. Then $\mathbf{T}_{-\mathbf{a}}\mathbf{T}\mathbf{0} = \mathbf{0}$, so $\mathbf{T}_{-\mathbf{a}}\mathbf{T} = \mathbf{O}$ is an element of $E(3)$ which leaves the origin invariant. Now it is clear that all $\mathbf{O} \in O(3)$, as constructed in the preceding section, are elements of $E(3)$ which leave the origin invariant. In fact $O(3)$ is a subgroup of $E(3)$. However, it is not so obvious that the elements of $O(3)$ are the *only* isometries that fix $\mathbf{0}$. In particular it is not obvious (but true) that every distance-preserving transformation of

R_3 that fixes $\mathbf{0}$ is necessarily a linear transformation, hence an element of $O(3)$. We assume this fact here and refer the reader to Yale [1] for a proof. Thus, every $\mathbf{T} \in E(3)$ can be written uniquely in the form

$$(2.4) \quad \mathbf{T} = \mathbf{T}_a \mathbf{O} = \{\mathbf{a}, \mathbf{O}\}, \quad \mathbf{O} \in O(3).$$

Conversely, every product of the form (2.4) defines an element of $E(3)$. Note that $\mathbf{T}_a = \{\mathbf{a}, \mathbf{E}\}$ and $\mathbf{O} = \{\mathbf{0}, \mathbf{O}\}$. The action of the elements of $E(3)$ on R_3 is given by

$$(2.5) \quad \{\mathbf{a}, \mathbf{O}\}\mathbf{x} = \mathbf{Ox} + \mathbf{a}, \quad \mathbf{x} \in R_3,$$

and the product rule is

$$(2.6) \quad \{\mathbf{a}_1, \mathbf{O}_1\}\{\mathbf{a}_2, \mathbf{O}_2\} = \{\mathbf{a}_1 + \mathbf{O}_1 \mathbf{a}_2, \mathbf{O}_1 \mathbf{O}_2\}.$$

Comparing this expression with (5.1) of Chapter 1, we see that $E(3)$ is a semi-direct product of $T(3)$ and $O(3)$. Indeed, the map $\mathbf{O} \rightarrow v_{\mathbf{O}}$, where $v_{\mathbf{O}}(\mathbf{a}) = \mathbf{Oa}$, is a homomorphism of $O(3)$ into the automorphism group of $T(3)$. One consequence of this result is that $T(3)$ is a normal subgroup of $E(3)$. The factor group $E(3)/T(3)$ is isomorphic to $O(3)$.

Suppose $\mathbf{T} \in E(3)$ leaves a point \mathbf{a} invariant, i.e., $\mathbf{T}(\mathbf{a}) = \mathbf{a}$. Then $\mathbf{T}_a^{-1}\mathbf{T}\mathbf{T}_a = \mathbf{O}$ leaves $\mathbf{0}$ invariant, so

$$(2.7) \quad \mathbf{T} = \mathbf{T}_a \mathbf{O} \mathbf{T}_a^{-1}, \quad \mathbf{O} \in O(3).$$

Conversely, any group element of the form $\mathbf{T}_a \mathbf{O} \mathbf{T}_a^{-1}$ leaves \mathbf{a} invariant. The reader should have no trouble in verifying that the elements (2.7) are rotations or rotation-inversions about axes through \mathbf{a} . All such elements clearly form a subgroup $O_a(3)$, the orthogonal group at \mathbf{a} . From (2.7) we have

$$(2.8) \quad O_a(3) = \mathbf{T}_a O(3) \mathbf{T}_a^{-1}.$$

The subgroup of rotations and rotation-inversions about \mathbf{a} is conjugate, hence isomorphic, to $O(3)$. A slight extension of this argument shows that all rotations by a fixed angle θ , $0 \leq \theta \leq \pi$, through any axis in R_3 form a single conjugacy class in $E(3)$. The same holds for all rotation-inversions by a fixed angle θ' .

We now give a geometrical interpretation of the elements of $E(3)$. First, consider the element $\{\mathbf{a}, C_k(\theta)\}$, where $\theta \neq 0$ and $\langle \mathbf{a}, \mathbf{k} \rangle = 0$, i.e., \mathbf{a} is perpendicular to the axis of rotation. This transformation has a fixed point \mathbf{b} . Indeed, the formula

$$\mathbf{T}_b^{-1}\{\mathbf{a}, \mathbf{O}\}\mathbf{T}_b = \{\mathbf{a} - \mathbf{b} + \mathbf{Ob}, \mathbf{O}\}$$

and the remarks preceding (2.7) show that $\{\mathbf{a}, C_k(\theta)\}$ leaves \mathbf{b} invariant if

$$(2.9) \quad \mathbf{b} - C_k(\theta)\mathbf{b} = \mathbf{a}.$$

Looking at a plane through \mathbf{a} and perpendicular to \mathbf{k} we have the situation shown in Fig. 2.1. There are an infinite number of solutions \mathbf{b} forming an axis

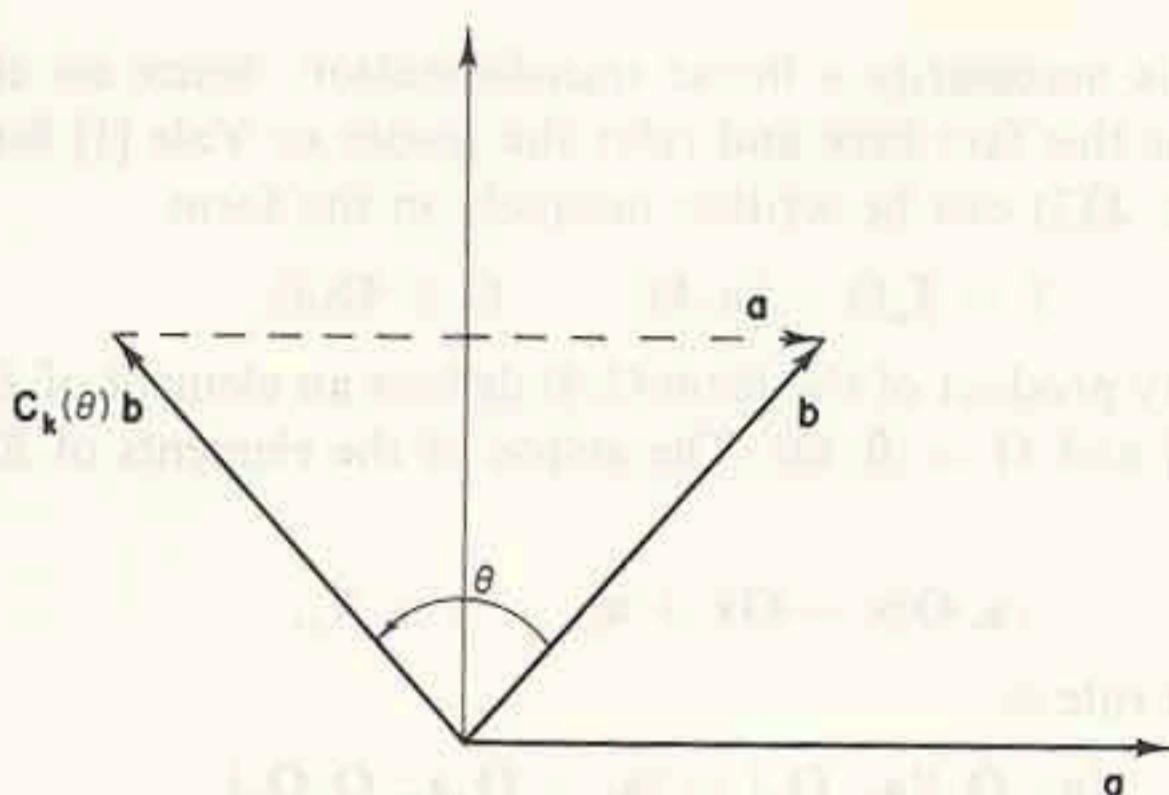


FIGURE 2.1

parallel to \mathbf{k} . Thus, $\{\mathbf{a}, \mathbf{C}_k(\theta)\}$ corresponds to a rotation through the angle θ about this invariant axis.

If \mathbf{a} is an arbitrary vector, we can write $\mathbf{a} = \mathbf{a}_1 + \mathbf{a}_2$ uniquely, where \mathbf{a}_1 is parallel to \mathbf{k} and \mathbf{a}_2 is perpendicular to \mathbf{k} . Then

$$(2.10) \quad \{\mathbf{a}, \mathbf{C}_k(\theta)\} = \mathbf{T}_{\mathbf{a}_1}\{\mathbf{a}_2, \mathbf{C}_k(\theta)\}.$$

The transformation (2.10) is called a **screw displacement**, a rotation through an angle θ about the **screw axis**, followed by a translation along the axis by a distance $\|\mathbf{a}_1\|$. (If we think of the rotation and translation as being performed simultaneously we get a right-handed screwing motion, which justifies the name.)

A similar analysis shows that the isometry

$$(2.11) \quad \{\mathbf{a}, \mathbf{S}_k(0)\} = \{\mathbf{a}, \sigma_k\}$$

is the product of the reflection in a plane perpendicular to \mathbf{k} , the **glide plane**, and a translation in this plane. This transformation is called a **glide reflection**.

Finally, the isometry

$$(2.12) \quad \{\mathbf{a}, \mathbf{S}_k(\theta)\}, \quad \theta \neq 2\pi n,$$

represents a rotation-inversion about some point. To see this we introduce a new rectangular coordinate system for R_3 centered at the origin and such that the vector \mathbf{k} points along the 3-axis. The transformation (2.12) maps the point $\mathbf{x} = (x_1, x_2, x_3)$ into $(x_1 \cos \theta - x_2 \sin \theta + a_1, x_1 \sin \theta + x_2 \cos \theta + a_2, a_3 - x_3)$. The reader can verify that this transformation has a unique fixed point \mathbf{x}_0 for $0 < \theta < 2\pi$. Thus, (2.12) must either be a rotation or a rotation-inversion about \mathbf{x}_0 and it is easy to show that it cannot be a rotation.

We have given geometrical interpretations for all elements of $E(3)$. The Euclidean group is made up of translations, rotations, rotation-inversions,

screw displacements, and glide reflections. (There is a slight overlap in this classification since, for example, there are degenerate screw displacements which are also rotations.) From another point of view, the above constitutes a list of conjugacy classes of $E(3)$. The reader should have no difficulty in showing that all translations through a distance d form a single conjugacy class, all screw displacements with angle θ and translation distance d form a single conjugacy class, and so on,

The map $\{\mathbf{a}, \mathbf{O}\} \rightarrow \det O$ defines a homomorphism of $E(3)$ onto the cyclic group of order two. The kernel of this homomorphism is $E^+(3)$, the **proper Euclidean group** in three-space or the **group of rigid motions**. Clearly, $E^+(3)$ is a normal subgroup of $E(3)$ and consists of all translations, rotations, and screw displacements. The elements of $E^+(3)$ are also called **direct isometries** or **direct symmetries**.

2.3 Symmetry and the Discrete Subgroups of $E(3)$

Let S be a subset of the space R_3 , and define

$$G = \{\mathbf{T} \in E(3) : \mathbf{T}S = S\},$$

the group of all elements of $E(3)$ that map S onto itself. We call G the **complete symmetry group** of S . Any subgroup of G is called a **symmetry group** of S . It is not required that any point of S be fixed under \mathbf{T} , merely that \mathbf{T} act as a permutation of the points of S . For example, the complete symmetry group of R_3 is $E(3)$. The complete symmetry group of a sphere with center at θ is $O(3)$. A right-pyramid-shaped figure with base given by Fig. 2.2 has C_2 , the

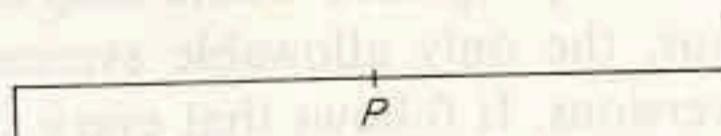


FIGURE 2.2

cyclic group of order two, as complete symmetry group. The elements of C_2 are the identity and a rotation of 180° about the axis through P perpendicular to the base. Of course, many subsets S are without symmetry, i.e., their complete symmetry groups consist of the identity element alone.

To find all possible symmetry groups it is necessary to classify all subgroups of $E(3)$. This is an extremely difficult problem! Fortunately, only two types of symmetry groups occur with much frequency in the physical sciences: discrete groups and Lie groups. These two types are easy to handle mathematically, which is one reason why they occur in applications. However, there are also good geometrical and physical reasons for limiting ourselves to such groups.

The groups $E(3)$, $O(3)$, $T(3)$, and C_∞ [the group of all rotations about a fixed axis, isomorphic to $SO(2)$] are examples of Lie groups. They will be studied in detail in subsequent chapters.

Definition. A discrete group G is a subgroup of the transformation group $E(3)$ such that for any $\mathbf{x} \in R_3$ and any sphere $B_r = \{\mathbf{y} \in R_3 : \|\mathbf{y}\| \leq r\}$ there are only a finite number of points in the G -orbit of \mathbf{x} that are contained in B_r .

If G is a discrete group then the points $G\mathbf{x} = \{\mathbf{y} = g\mathbf{x} : g \in G\}$ are distributed in R_3 so that only a finite number of them are contained in each bounded subset of R_3 . Clearly, every finite subgroup of $E(3)$ is discrete since every G -orbit of a finite group contains only a finite number of elements. The group of all translations $\{\mathbf{T}_a\}$ where

$$(3.1) \quad \mathbf{a} = a_1 \mathbf{e}_1 + a_2 \mathbf{e}_2 + a_3 \mathbf{e}_3$$

and a_1 , a_2 , and a_3 are integers is an infinite discrete group. On the other hand the group of all translations $\{\mathbf{T}_a\}$ where \mathbf{a} takes the form (3.1) with a_1 , a_2 , and a_3 rational is neither a Lie group or a discrete group. Another infinite nondiscrete group is generated by a rotation through the angle $2\pi/a$ about an axis, where a is not a rational number. (Prove it!)

Let us search for the possible discrete symmetry groups of objects (or sets) of finite extent, i.e., objects which can be wholly contained inside some sufficiently large sphere B_r . Clearly such symmetry groups cannot contain nontrivial translations, screw displacements, or glide reflections since one of these transformations indefinitely repeated would map the object outside of the bounding sphere. Thus, the only allowable symmetry operations are rotations and rotation-inversions. It follows that every symmetry of a finite object has at least one fixed point. However, it is not so obvious that the symmetries have a common fixed point.

Theorem 2.3. Let S be a nonempty set of finite extent and let G be a discrete symmetry group of S . Then there is at least one point $\mathbf{y} \in R_3$ which is fixed by all $\mathbf{g} \in G$.

Proof. Since S is bounded it can be enclosed inside some sphere B_r . Let $\mathbf{x} \in S$ and consider the G -orbit containing \mathbf{x} . All points in this G -orbit must be in S , hence in B_r . Since G is discrete it follows that the orbit is finite:

$$G\mathbf{x} = \{\mathbf{x}_1 = \mathbf{x}, \mathbf{x}_2, \dots, \mathbf{x}_n\}.$$

Let

$$(3.2) \quad \mathbf{y} = \left(\sum_{i=1}^n \mathbf{x}_i \right) / n$$

be the **centroid** of Gx . Since the action of an element of $E(3)$ on R_3 is given by (2.5) it follows easily that

$$(3.3) \quad gy = \left(\sum_{i=1}^n gx_i \right) / n, \quad g \in G,$$

i.e., the centroid of the finite set $\{x_i\}$ is mapped onto the centroid of $\{gx_i\}$ for any $g \in G$. On the other hand, the transformation g merely permutes the elements of the G -orbit through x . Thus, the terms on the right-hand sides of (3.2) and (3.3) are equal except for order, and the sums are the same. We conclude that $gy = y$, so the centroid y is a common fixed point for all symmetries of S .

Corollary 2.1. The elements of a finite subgroup of $E(3)$ have a common fixed point.

Theorem 2.4. Let G be a discrete subgroup of $E(3)$ whose elements have a common fixed point y . Then G is a finite subgroup of the orthogonal group $O(3)$ of rotations and rotation-inversions about y .

Proof. Let x_1, \dots, x_4 be four noncoplanar points lying within a sphere B_r with center y . Since $\|gx_i - y\| = \|gx_i - gy\| = \|x_i - y\|$, the orbits $\{Gx_i\}$ all lie inside B_r . Since G is discrete, there are only a finite number of points in these G -orbits. Now the transformation $g \in G$ is uniquely determined by the four noncoplanar points $\{gx_i\}$. For, if $gx_i = g'x_i$, $1 \leq i \leq 4$, then the $\{x_i\}$ are invariant under $g^{-1}g'$, so $g^{-1}g' = E$, the identity operator. [An element of $E(3)$ is uniquely determined by its action on the $\{x_i\}$.] Hence, $g' = g$ and our argument shows that G is a finite group. Q.E.D.

Thus, a discrete symmetry group of a body S of finite extent is always a finite group G of rotations and rotation-inversions about some fixed point y . If we consider $O(3)$ as the orthogonal group with fixed point θ , it is clear that G is conjugate to the finite subgroup $T_y^{-1}GT_y = K$ of $O(3)$, and K is a symmetry group of $T_y^{-1}S$. Similarly, if $T \in E(3)$ with $T\theta = y$ then TKT^{-1} is a finite group of rotations and rotation-inversions with fixed point y . To simplify the classification of symmetry groups we will identify conjugate subgroups of $E(3)$. Conjugate symmetry groups are physically indistinguishable. Our listing of symmetry groups will really be a listing of equivalence classes of conjugate subgroups.

In abstract group theory, one identifies two groups if they are isomorphic, i.e., if they have the same multiplication table. This is not the same as the classification into conjugate subgroups of $E(3)$. Conjugate subgroups are isomorphic, but isomorphic subgroups of $E(3)$ need not be conjugate. For example, the cyclic groups of order two generated by a rotation of 180° about

an axis and a reflection in a plane, respectively, are isomorphic but not conjugate.

To recapitulate, the problem of classifying all discrete symmetry groups of objects of finite extent reduces to the problem of listing all finite subgroups of $O(3)$. [It is obvious that each finite subgroup of $O(3)$ is the symmetry group of some object.] Subgroups of the transformation group $O(3)$ are called **point groups** since they always have a fixed point. (Without loss of generality we can assume that this fixed point is Θ .) These groups are of two types: point groups of the **first kind**, which contain only rotations, and point groups of the **second kind**, which also contain rotation-inversions.

To a great extent the problem of classifying point groups can be reduced to the problem of classifying point groups of the first kind. Let G be a finite point group and consider the homomorphism $g \rightarrow \det g$, $g \in G$ which maps G into the cyclic group of order two, i.e., g maps to $+1$ if it is a rotation and to -1 if it is a rotation-inversion. If the kernel of this homomorphism is G then G is a point group of the first kind. If the kernel is K , a proper subgroup of G , then by Theorems 1.4 and 1.5, K is a normal subgroup with half as many elements as G . Furthermore, the coset decomposition of G is $\{K, g_0K = Kg_0\}$. The elements of K are rotations and the elements of g_0K , including g_0 itself, are rotation-inversions. There are two possibilities: either G contains the inversion $I = -E$ or it does not. If $I \in G$ then $I \in g_0K$, so $IK = g_0K$ and we can take $g_0 = I$. Conversely, if K is a finite rotation group then the set $\{K, IK\}$ forms a point group of the second kind. If $I \notin G$ then the description of G becomes a little more complicated. Let

$$K^+ = \{Ig : g \in G, g \notin K\}.$$

It is easy to check that (1) the set K^+ consists of proper rotations, (2) $K^+ \cap K$ is empty, and (3) K^+ and K contain the same number of elements. In particular, (2) follows from the fact that $I \notin G$. Now let $G^+ = K \cup K^+$. We will show that G^+ is a point group of the first kind isomorphic to G . The isomorphism is the identity on K and maps $g \notin K$ into $Ig \in K^+$. This map is a homomorphism because I commutes with all group elements. Indeed the elements of G^+ can be written in the form $I^\varepsilon g$ for $g \in G$, where $\varepsilon = 0$ if $g \in K$ and $\varepsilon = 1$ if $g \notin K$. Then

$$(I^{\varepsilon_1}g_1)(I^{\varepsilon_2}g_2) = I^{\varepsilon_1 + \varepsilon_2}g_1g_2,$$

where $I^{\varepsilon_1 + \varepsilon_2} = E$ if $g_1g_2 \in K$, and is equal to I otherwise; which proves that the map is a homomorphism. Note that K is a normal subgroup of G^+ of index two. We have proved the following result.

Theorem 2.5. Let G be a finite subgroup of $O(3)$ and let $K = G \cap SO(3)$, the subgroup of rotations in G . There are exactly three possibilities: (1)

$G = K$, (2) $G = K \cup IK$, (3) $G \neq K, I \notin G$. In the last case G is isomorphic to the group of rotations $G^+ = K \cup K^+$.

Theorem 2.5 tells us how to construct all point groups of the second kind once we are given all point groups of the first kind. The only nontrivial constructions are in class (3), where we have to determine all point groups of the first kind G^+ that contain a normal subgroup K of index two. The point group G is then defined by means of the isomorphism discussed in the proof of the theorem.

2.4 Point Groups of the First Kind

Let G be a finite subgroup of $SO(3)$ with order $n(G) \geq 2$. Then G acts as a transformation group in Euclidean space whose elements have the origin $\mathbf{0}$ as a common fixed point. Let B_r be a sphere in R_3 , with center at the origin and radius $r > 0$. The elements of G clearly map the surface S_r of the sphere onto itself. A point \mathbf{x} on S_r is said to be a **pole** if $g\mathbf{x} = \mathbf{x}$ for some $g \in G$, not the identity element. That is, a pole is a point of intersection of S_r and the axis of a nontrivial rotation in G . Clearly, each element of G except the identity is associated with two poles. The transformation group G maps poles into poles. Indeed, if \mathbf{x} is a pole associated with g_1 , then $g_2\mathbf{x}$ is a pole associated with $g_2g_1g_2^{-1}$. It follows that the set of poles on S_r is partitioned into G -orbits. According to Theorem 1.6 the number of poles in the orbit containing \mathbf{x} is $p = n(G)/n(G^x)$, where G^x is the isotropy subgroup of G corresponding to \mathbf{x} , i.e., G^x is the subgroup of all rotations with pole \mathbf{x} . Suppose there are k orbits. Choosing a point \mathbf{x}_i in each orbit we see that the number of nontrivial rotations with pole \mathbf{x}_i is $n_i - 1 = -1 + n/p_i$, where $n = n(G)$, $n_i = n(G^{x_i})$, and p_i is the number of poles in the i th orbit. (Recall that n_i is the same for all points in the i th orbit.). We have subtracted 1 since the identity element in G^{x_i} is a trivial rotation. The total number of rotations leaving some pole in the i th orbit fixed is thus $p_i(n_i - 1)$. Summing over the orbits, we find that the total number of rotations leaving some pole fixed is $\sum_{i=1}^k p_i(n_i - 1)$. Since each rotation is associated with two poles this sum equals $2(n - 1)$, i.e., each nontrivial rotation is counted twice. Thus we have the identity

$$(4.1) \quad 2(1 - 1/n) = \sum_{i=1}^k (1 - 1/n_i),$$

where $n \geq n_i \geq 2$. This equation can be solved only if $2 \leq k \leq 3$. If $k = 2$ then (4.1) becomes

$$(4.2) \quad 2/n = 1/n_1 + 1/n_2.$$

Furthermore, (4.2) can be solved if and only if $n_1 = n_2 = n$, $n = 2, 3, \dots$

Thus, the finite rotation groups G with two orbits are associated with two poles, each pole fixed by all elements of G . There is only one axis of rotation.

The cyclic groups C_n of order n ($n = 2, 3, \dots$) generated by a rotation through the angle $2\pi/n$ about a fixed axis clearly satisfy the above requirements. We shall show that these are the only point groups of the first kind whose poles can be partitioned into two orbits.

Lemma 2.2. Let G be a group of order $n \geq 2$ consisting of rotations about a fixed axis. Then $G \cong C_n$.

Proof. The n elements e, g_1, \dots, g_{n-1} of G correspond to rotations through the angles $0, \theta_1, \dots, \theta_{n-1}$ about the fixed axis, where 0 corresponds to the identity element. We can assume $0 < \theta_i < 2\pi$, $1 \leq i \leq n - 1$, if the rotation angles are expressed in radians, and renumber the elements of G so that θ_1 is the smallest positive rotation angle. Using the Euclidean algorithm we see that for each θ_i , $2 \leq i \leq n - 1$, there is an integer m_i such that

$$\theta_i = m_i \theta_1 + \varphi_i, \quad 0 \leq \varphi_i < \theta_1.$$

But $g_i g_1^{-m_i} \in G$, so φ_i is the rotation angle of some element of G . Since θ_1 is the smallest positive rotation angle, the only possibility is $\varphi_i = 0$. Thus G is a cyclic group generated by g_1 . Since G has order n it follows that $\theta_1 = 2\pi/n$. Q.E.D.

We now return to the solution of (4.1) for $k = 3$,

$$(4.3) \quad 1 + 2/n = 1/n_1 + 1/n_2 + 1/n_3, \quad n \geq n_i \geq 2.$$

It can be assumed that $n_1 \leq n_2 \leq n_3$. Clearly, there is no solution for $3 \leq n_1$ since in that case

$$1 + 2/n > 1 \geq 1/n_1 + 1/n_2 + 1/n_3.$$

Therefore $n_1 = 2$. If $n_2 = 2$ we get the unique solution

$$(a) \quad n_1 = n_2 = 2, \quad n_3 = n/2, \quad n \text{ even}, \quad n \geq 4.$$

If $n_2 \geq 4$ there is no solution since

$$1 + 2/n > 1 \geq \frac{1}{2} + \frac{1}{4} + 1/n_3, \quad n_3 \geq 4.$$

Thus, the only remaining possibility is $n_2 = 3$:

$$1/6 + 2/n = 1/n_3, \quad n \geq n_3 \geq 3, \quad 6 > n_3.$$

The possible solutions are

$$(b) \quad n_1 = 2, \quad n_2 = n_3 = 3, \quad n = 12,$$

$$(c) \quad n_1 = 2, \quad n_2 = 3, \quad n_3 = 4, \quad n = 24,$$

$$(d) \quad n_1 = 2, \quad n_2 = 3, \quad n_3 = 5, \quad n = 60.$$

This exhausts the solutions of (4.1). We will show that each of the solutions (a)–(d) uniquely defines a point group of the first kind.

In solution (a) set $n = 2m$, $m \geq 2$ an integer. There is a rotation axis corresponding to a rotation subgroup of order m . It follows from Lemma 2.2 that this subgroup is C_m and is generated by the rotation through the angle $2\pi/m$ about the fixed axis L . We say L is an **m -fold** axis. The poles of L lie in the same orbit. We have now determined m elements of the point group. To get the remaining elements, note that there are m twofold axes of rotation, l_1, \dots, l_m whose poles are divided into two orbits of m poles each. Since the two poles of L form a single orbit, each of the rotations by π radians about a twofold axis l_i must interchange the poles. Thus the two-fold axes are perpendicular to L . A rotation by $2\pi/m$ about L maps the l_i into themselves. By considering rotations about twofold axes we can easily show that the angle between two adjacent l_i in the plane perpendicular to L is a fixed constant. Thus, the angle between any two adjacent l_i must be π/m .

The abstract structure of the transformation group corresponding to (a) is now uniquely determined. Let \mathbf{C} be the rotation of $2\pi/m$ about L and let τ be a rotation by π about one of the twofold axes. Since the cyclic group C_m generated by \mathbf{C} has order m , it follows that the elements of G can be divided into two cosets C_m and τC_m . The m elements in the second coset are of order two since they interchange the poles of L . Thus, $\tau^{-1} = \tau$ and $(\tau \mathbf{C})^2 = \mathbf{e}$, or

$$(4.4) \quad \tau \mathbf{C} = \mathbf{C}^{-1} \tau.$$

Any element g of G can be written uniquely in the form

$$(4.5) \quad g = \tau^\varepsilon \mathbf{C}^k, \quad \varepsilon = 0, 1, \quad k = 0, 1, \dots, m-1.$$

The multiplication of two group elements is then uniquely determined by (4.4). For example,

$$(4.6) \quad (\tau \mathbf{C}^{k_1})(\tau \mathbf{C}^{k_2}) = \mathbf{C}^{k_2 - k_1}, \quad (\tau \mathbf{C}^{k_1})(\mathbf{C}^{k_2}) = \tau \mathbf{C}^{k_1 + k_2}.$$

The abstract group defined by these rules is denoted D_m , the **dihedral group** of order $2m$.

We will list the conjugacy classes of D_m since they are of importance for representation theory. The details in the straightforward proofs will be left to the reader. Because of the presence of rotations which interchange the poles of L , the rotations \mathbf{C}^k and $\mathbf{C}^{-k} = \mathbf{C}^{m-k}$, $k = 1, \dots, m-1$, are conjugate. (The axis L is called **two-sided** because both poles of L lie in the same orbit.) Since C_m is a normal subgroup of D_m the conjugacy classes $\{\mathbf{C}^k, \mathbf{C}^{m-k}\}$ contain no elements not in C_m . There are $1 + (m/2)$ such classes if m is even and $(m+1)/2$ classes if m is odd. The m rotations τ_1, \dots, τ_m about the two-fold axes form a single conjugacy class if m is odd and two classes if m is

even. Thus D_m has a total of $(3 + m)/2$ classes for odd m and $3 + (m/2)$ classes for even m .

For each m we shall exhibit a solid with D_m as its largest point symmetry group of the first kind. An **m -prism** is a right cylinder with base a regular m -sided polygon and height not equal to one side of the polygon. In the case $m = 2$ we define a regular two-sided polygon as a plane figure looking as shown in Fig. 2.3. The reader can check that D_m is a symmetry group of the

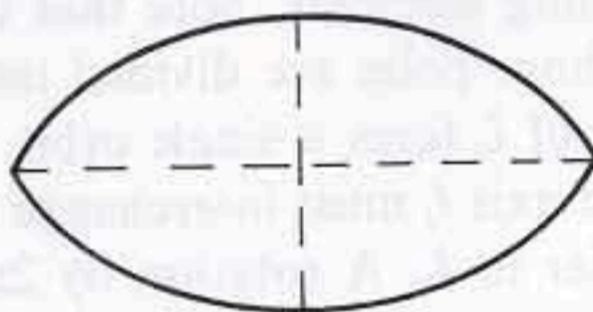


FIGURE 2.3

m -prism. In particular the axis L of the m -prism is the m -fold axis and the midpoint of L is invariant under all elements of D_m . Similarly, it is easy to show that C_m is the maximal direct symmetry group of an **m -pyramid**. An m -pyramid is a right pyramid with base a regular m -sided polygon such that the distance from the vertex of the pyramid to a vertex of the base is not equal to one side of the polygon.

Next we consider solution (b) of (4.1). There are four threefold axes L_1, \dots, L_4 , three twofold axes l_1, l_2, l_3 . Let $\{x_1, \dots, x_4\}$ be the poles in one of the orbits which contains four elements. The elements of G permute these poles transitively and effectively (since a nontrivial rotation can fix at most two poles). Any pole x_1 , say, is fixed by a cyclic subgroup C_3 of order three. It follows that for $2 \leq i < j \leq 4$ there exists $g \in C_3$ such that $gx_1 = x_1, gx_i = x_j$. Therefore, for distinct i, j, k there is a $g \in G$ such that $gx_i = x_i, gx_j = x_k$, i.e., the line segment $[x_i, x_j]$ is mapped onto $[x_i, x_k]$ by the rotation g . Thus, the poles x_1, \dots, x_4 are spaced equidistant from one another on the sphere S , and the tetrahedron with these poles as vertices admits G as a symmetry group. Clearly, G is a subgroup of the **tetrahedral group** T of all direct symmetries of the tetrahedron. However, $n(T) = 12$, so $G = T$. Indeed, every symmetry of the tetrahedron can be represented uniquely as a permutation of the four vertices x_1, \dots, x_4 . Out of the 24 possible permutations in S_4 , the reader can easily verify that only a subgroup of order 12, the even permutations, correspond to direct symmetries of the tetrahedron. The four threefold axes pass through the four vertices of the tetrahedron, while the three twofold axes join the midpoints of nonintersecting edges. There are four conjugacy classes: the identity, four rotations by 120° , four rotations by 240° , and three rotations by 180° .

Solution (c) of (4.1) corresponds to three fourfold axes L_1, L_2 , and L_3 ,

four threefold axes, and six twofold axes. All axes are two-sided. Consider the orbit with six poles (the poles of the L_i axes). G acts transitively and effectively on the poles of this orbit. Exactly two of the poles, say \mathbf{x}_1 and \mathbf{x}_2 , are fixed under the subgroup C_4 of rotations about the axis L_1 containing \mathbf{x}_1 and \mathbf{x}_2 . The four remaining poles are permuted by the elements of C_4 . Since C_4 contains an element of order four it follows that for $3 \leq i \leq j \leq 6$ there is a $\mathbf{g} \in C_4$ such that $\mathbf{g}\mathbf{x}_k = \mathbf{x}_k$, $k = 1, 2$, and $\mathbf{g}\mathbf{x}_i = \mathbf{x}_j$. Thus \mathbf{g} maps the line segments $[\mathbf{x}_1, \mathbf{x}_i]$ and $[\mathbf{x}_2, \mathbf{x}_i]$ onto $[\mathbf{x}_1, \mathbf{x}_j]$ and $[\mathbf{x}_2, \mathbf{x}_j]$, respectively. The distance between any two poles not on the same axis is a fixed constant, so the three L -axes are mutually orthogonal. Thus, we can construct a cube \mathcal{C} such that the six poles form the midpoints of the six faces of \mathcal{C} . The group G is obviously a subgroup of the **octahedral group** O , the direct symmetry group of \mathcal{C} . The reader can verify that $n(O) = 24$, so $G = O$. As we have mentioned, the three fourfold axes pass through the midpoints of the faces of \mathcal{C} . The four threefold axes pass through the vertices of \mathcal{C} and the six twofold axes pass through the midpoints of the edges of \mathcal{C} . The octahedral group contains five conjugacy classes. Since all axes are two-sided, the three rotations of 90° and the three rotations of 270° about the L_i form a single class, as do the four rotations of 120° and four rotations of 240° about the threefold axes. The remaining classes contain the identity, the three rotations of 180° about the L_i , and the six rotations of 180° about the twofold axes, respectively.

The octahedral group O is also the direct symmetry group of the octahedron, a figure formed by connecting the midpoints of adjacent faces of \mathcal{C} with straight lines. The octahedron is a regular polyhedron with 8 triangular faces, 12 edges, and 6 vertices.

Solution (d) of (4.1) corresponds to six fivefold axes L_1, \dots, L_6 , ten threefold axes, and fifteen twofold axes. All axes are two-sided. The 12 poles of the L_i axes lie in a single orbit. The transformation group G permutes these poles transitively and effectively. Let us choose an axis L_1 with poles $\mathbf{x}_1, \mathbf{x}_2$. The subgroup of rotations that fix each of $\mathbf{x}_1, \mathbf{x}_2$ is isomorphic to C_5 . In particular the rotation \mathbf{g} through the angle 72° about L_1 is an element of order five. The action of \mathbf{g} on the orbit can thus be represented by the permutation

$$(4.7) \quad (\mathbf{x}_3 \mathbf{x}_4 \cdots \mathbf{x}_7)(\mathbf{x}_8 \mathbf{x}_9 \cdots \mathbf{x}_{12})$$

if the poles are suitably labeled. This is the only possibility since \mathbf{g} must have order five and leave none of the poles $\mathbf{x}_3, \dots, \mathbf{x}_{12}$ fixed. Therefore, under the action of C_5 , the single G -orbit splits into four C_5 -orbits: two fixed poles and two orbits containing five poles each.

Think of \mathbf{x}_1 and \mathbf{x}_2 as the north and south poles of the sphere B_r . The remaining poles $\mathbf{x}_3, \dots, \mathbf{x}_{12}$ cannot all lie on the equator since then a rotation through 72° about one of the axes L_i , $2 \leq i \leq 6$, would map some of the

\mathbf{x}_i into points which are neither on the equator or at the north or south poles. This is impossible because the G -orbit contains only 12 elements. Therefore, without loss of generality we can assume that \mathbf{x}_3 is in the northern hemisphere. There must then be five poles in the northern hemisphere since rotations by 72° about L_1 map \mathbf{x}_3 into $\mathbf{x}_4, \dots, \mathbf{x}_7$, successively. The five remaining poles are in the southern hemisphere since they lie on the other ends of axes through the poles $\mathbf{x}_3, \dots, \mathbf{x}_7$. Our original choice of the axis L_1 was arbitrary, so we have established that each pole has five nearest-neighbor poles, five distant poles, and its antipode. The distance between nearest-neighbor poles is a fixed constant.

Now draw straight lines connecting each pole to its five nearest neighbors. The figure thus formed, assuming it exists, is a regular polyhedron with 12 vertices (the poles), 30 edges, and 20 faces. (Prove it!) The faces are equilateral triangles.

Such a regular polyhedron does exist. It is called the icosahedron and the dubious reader can construct it by gluing 20 congruent equilateral triangles together along the edges. The direct symmetry group of the icosahedron is the **icosahedral group** Y . Clearly G is a subgroup of Y . It is easy to enumerate the possible direct symmetries of the icosahedron. The only possible axes are: 6 fivefold axes through pairs of opposite vertices, 10 threefold axes through the midpoints of opposite faces, and 15 twofold axes through the midpoints of opposite edges. Thus Y contains a total of 60 elements. Since $n(G) = 60$ it follows that $G = Y$.

There are five conjugacy classes in Y : the class of the identity element, the class containing 15 rotations of 180° , the class containing 10 rotations of 120° and 10 rotations of 240° , the class containing 6 rotations of 72° and 6 rotations of 288° , and the class containing 6 rotations of 144° and 6 rotations of 216° .

The icosahedral group is also the direct symmetry group of the dodecahedron. This regular polyhedron can be obtained by joining with straight lines the midpoints of adjacent faces of the icosahedron. The dodecahedron has 20 vertices and 30 edges. Its 12 faces are regular pentagons.

We have shown that a complete list of point groups of the first kind is given by the cyclic groups C_m , the dihedral groups D_m , $m \geq 2$, the tetrahedral group T , the octahedral group O , and the icosahedral group Y . No two groups in this list are isomorphic.

2.5 Point Groups of the Second Kind

A list of point groups of the second kind can be obtained from Theorem 2.5 and results of the last section. First we list all groups generated by the inversion **I** and a point group of the first kind K . Clearly $n(G) = 2n(K)$. As

an abstract group G is isomorphic to the direct product $K \times H = K \cup \mathbf{IK}$, where H is the group with two elements $\{\mathbf{E}, \mathbf{I}\}$. Thus, the multiplication table for G can be obtained in an obvious way from the multiplication table for K . The number of conjugacy classes for G is just twice the number for K . The list is as follows:

(1) $C_n \cup \mathbf{IC}_n$. This is an abelian group of order $2n$ consisting of all rotations through multiples of the angle $2\pi/n$ about a fixed axis and all such rotations followed by an inversion. The group has $2n$ conjugacy classes, each class containing one element. For n odd there is an isomorphism $C_{2n} \cong C_n \cup \mathbf{IC}_n$. However, these two groups are not conjugate subgroups of $E(3)$. Also, $D_2 \cong C_2 \cup \mathbf{IC}_2$, but again the two subgroups are not conjugate.

(2) $D_n \cup \mathbf{ID}_n$, $n \geq 2$. This group of order $4n$ has $3 + n$ conjugacy classes if n is odd and $6 + n$ if n is even. For odd $n \geq 3$ there is an isomorphism $D_n \cup \mathbf{ID}_n \cong D_{2n}$, but the two subgroups are not conjugate.

(3) $T \cup \mathbf{IT} = T_h$. The group T_h is of order 24 and contains 8 conjugacy classes.

(4) $O \cup \mathbf{IO} = O_h$. The group O_h is the complete symmetry group of the cube. It has order 48 and contains 12 conjugacy classes.

(5) $Y \cup \mathbf{IY} = Y_h$. This is the complete symmetry group of the icosa-hedron. It contains 120 elements divided into 10 conjugacy classes.

Next we construct the groups mentioned in part (3) of Theorem 2.6. We look for all point groups G^+ of the first kind such that G^+ contains a subgroup K of index two. With $G^+ = K \cup K^+$ it follows that $G = K \cup \mathbf{IK}^+$ is a point group of the second kind isomorphic (but not conjugate) to G^+ . Examining our list of point groups of the first kind we find the possibilities given in Table 2.1. Perhaps the easiest way to obtain these results is to search

TABLE 2.1

	G^+	K	Order of G	Number of conjugacy classes
(6)	C_{2n}	C_n	$2n$	$2n$
(7)	D_n	C_n , $n \geq 2$	$2n$	$\begin{cases} (3+n)/2, & n \text{ odd} \\ 3+(n/2), & n \text{ even} \end{cases}$
(8)	D_{2n}	D_n , $n \geq 2$	$4n$	$3+n$
(9)	O	T	24	5

for all homomorphisms of G^+ onto the cyclic group of order two. An element of odd order in G^+ is necessarily in the kernel K of each homomorphism. Only the elements of even order have to be examined with special care.

Since $G \cong G^+$, the multiplication table and the number of conjugacy classes for G are the same as for G^+ . However, G and G^+ act differently as

transformation groups because one group contains rotation-inversions and the other does not.

The group of type (9) is usually denoted as T_d in Schöenflies notation (Hamermesh [1]). T_d contains T as a normal subgroup and is the complete symmetry group of the tetrahedron. The groups of type (7) are denoted C_{nv} , $n = 2, 3, \dots$. The C_{nv} group is the complete symmetry group of an n -pyramid. It contains the subgroup C_n of rotations about the vertical n -fold axis of the pyramid as well as reflections in n vertical planes passing through this axis.

The groups of types (1), (2), (6), and (8) are classified in a different manner by Schöenflies. The type (1) group for odd n and the type (6) group for even n are lumped together to form the cyclic group S_{2n} of order $2n$. A generator of S_{2n} is given by the rotation-inversion $S(\pi/n)$, i.e., a rotation of π/n about an axis followed by reflection in a plane perpendicular to the axis. The even powers of $S(\pi/n)$ form the subgroup C_n . The type (1) group for even n and the type (6) group for odd n are combined to form the abelian group C_{nh} , which consists of the $2n$ rotations and rotation-inversions about a fixed axis by all multiples of $2\pi/n$.

The type (2) group for even n and the type (8) group for odd n form D_{nh} , the complete symmetry group of the n -prism. This group of order $4n$ contains C_{nh} as a subgroup of order $2n$. The type (2) group for odd n and the type (8) group for even n form D_{nd} of order $4n$. The group D_{nd} is the complete symmetry group of a **twisted n -prism**, obtained by joining together two n -prisms at their bases in such a way that the prisms are rotated relative to one another by the angle π/n . Here, D_{nd} contains S_{2n} as a subgroup.

We have not listed solids whose complete symmetry groups are T_h , S_{2n} , and C_{nh} . Such solids are not difficult to construct, however, and we refer the interested reader to Yale [1].

2.6 Lattice Groups

A **lattice group** G is a nontrivial discrete subgroup of $T(3)$, the translation group in three-space. By nontrivial we mean that G is not just the identity element. Since the elements $\mathbf{T}_\mathbf{a}$ of $T(3)$ are completely determined by the 3-vectors $\mathbf{a} = \alpha_1 \mathbf{e}_1 + \alpha_2 \mathbf{e}_2 + \alpha_3 \mathbf{e}_3$, we can think of G as a group of 3-vectors \mathbf{a} whose law of group multiplication is vector addition:

$$\mathbf{T}_{\mathbf{a}_1} \mathbf{T}_{\mathbf{a}_2} = \mathbf{T}_{\mathbf{a}_1 + \mathbf{a}_2}.$$

If the vector group G contains three linearly independent vectors it is said to be **three-dimensional**. If G contains only two linearly independent vectors, i.e., if all the vectors lie in a plane through $\mathbf{0}$, then G is **two-dimensional**. If all the vectors lie on a line through $\mathbf{0}$, then G is **one-dimensional**. If $\mathbf{a}_1, \dots, \mathbf{a}_k$

are linearly independent vectors in a k -dimensional lattice group then every $\mathbf{a} \in G$ can be written uniquely in the form

$$(6.1) \quad \mathbf{a} = \alpha_1 \mathbf{a}_1 + \cdots + \alpha_k \mathbf{a}_k,$$

where the α_i are real numbers. We shall be primarily concerned with three-dimensional lattice groups and we shall always consider G as a group of vectors under addition. In this way we obtain a geometrical model of each lattice group.

Two linearly independent vectors \mathbf{a}_1 and \mathbf{a}_2 in a lattice group determine a parallelogram with vertices $\mathbf{0}$, \mathbf{a}_1 , \mathbf{a}_2 , and $\mathbf{a}_1 + \mathbf{a}_2$ (all in G) (Fig. 2.4).

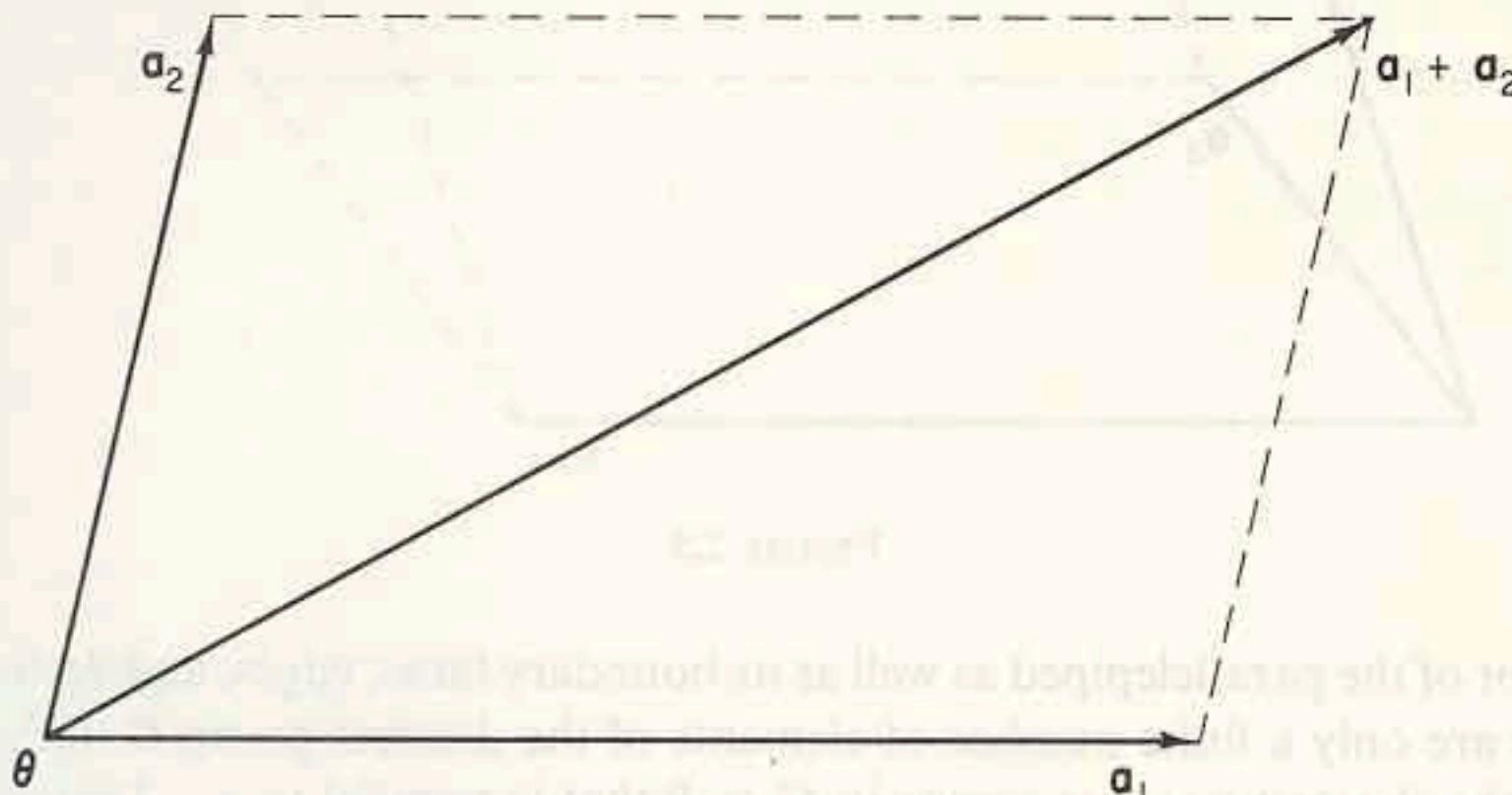


FIGURE 2.4

Similarly, three linearly independent vectors \mathbf{a}_1 , \mathbf{a}_2 , and \mathbf{a}_3 determine a parallelepiped with vertices $\mathbf{0}$, \mathbf{a}_1 , \mathbf{a}_2 , \mathbf{a}_3 , $\mathbf{a}_1 + \mathbf{a}_2$, $\mathbf{a}_1 + \mathbf{a}_3$, $\mathbf{a}_2 + \mathbf{a}_3$, and $\mathbf{a}_1 + \mathbf{a}_2 + \mathbf{a}_3$ in G (Fig. 2.5).

The following theorem exhibits the structure of three-dimensional lattice groups and justifies the term "lattice." If \mathbf{a}_1 , \mathbf{a}_2 , and \mathbf{a}_3 are linearly independent then the set $\{\alpha_1 \mathbf{a}_1 + \alpha_2 \mathbf{a}_2 + \alpha_3 \mathbf{a}_3\}$, where the α_i run over all possible integers, is clearly a subgroup of G . We show it is possible to choose the \mathbf{a}_i so this set is all of G .

Theorem 2.6. Let G be a three-dimensional lattice group. Then there exist linearly independent vectors \mathbf{b}_1 , \mathbf{b}_2 , \mathbf{b}_3 in G such that every $\mathbf{a} \in G$ can be written uniquely in the form

$$(6.2) \quad \mathbf{a} = n_1 \mathbf{b}_1 + n_2 \mathbf{b}_2 + n_3 \mathbf{b}_3$$

where the n_i are integers.

Proof. Let \mathbf{a}_1 , \mathbf{a}_2 , \mathbf{a}_3 be linearly independent vectors in G and let P be the cell in R_2 determined by these vectors. (We think of P as consisting of the

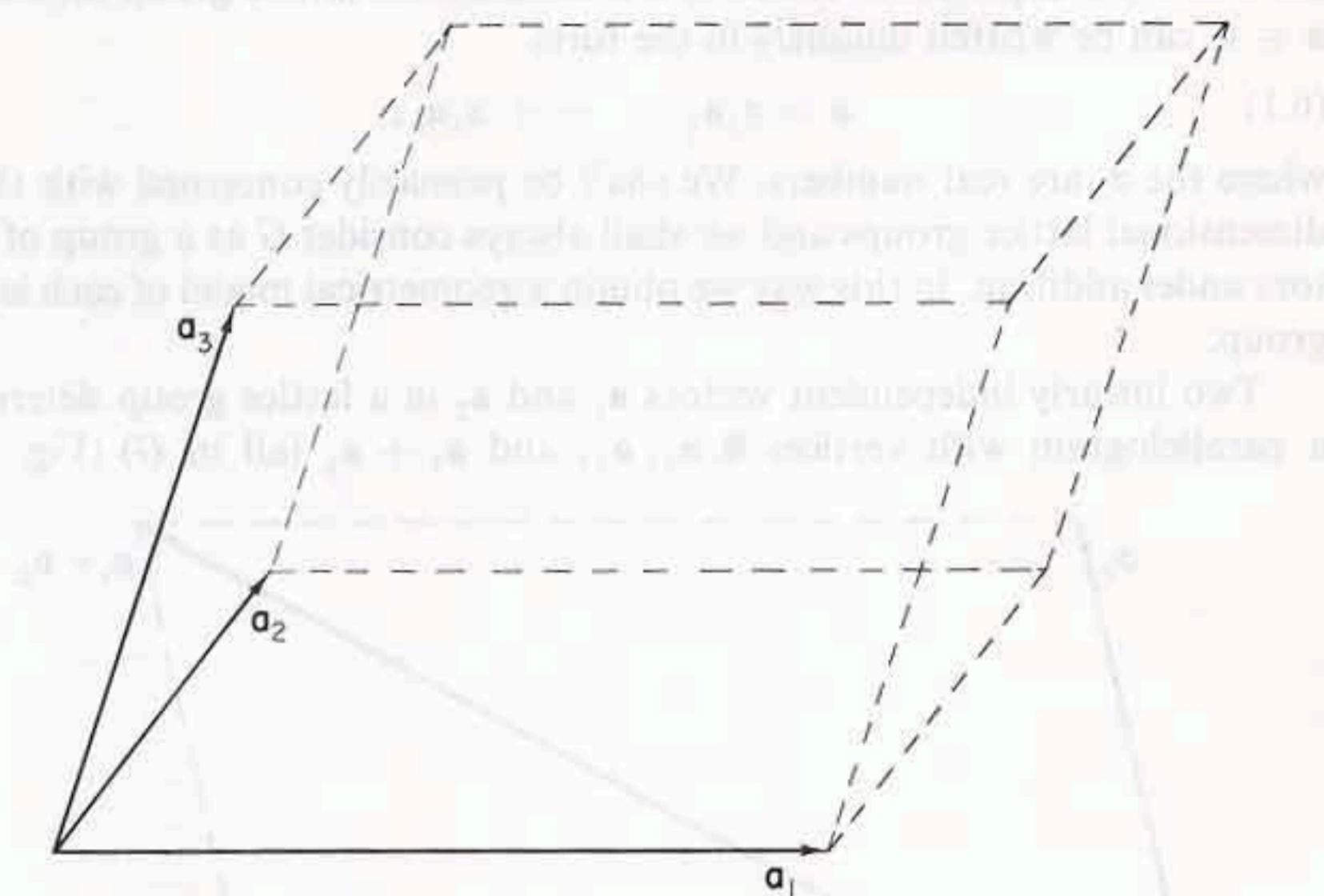


FIGURE 2.5

interior of the parallelepiped as well as its boundary faces, edges, and vertices.) There are only a finite number of elements of the discrete group G in P . Let \mathbf{b}_1 be the shortest nonzero vector in $G \cap P$ that is parallel to \mathbf{a}_1 . That is, on the edge of P with endpoints $\mathbf{0}$ and \mathbf{a}_1 , we choose the element $\mathbf{b}_1 \neq \mathbf{0}$ of G closest to $\mathbf{0}$. Now let \mathbf{b}_2 be an element of G in the parallelogram generated by $\mathbf{a}_1, \mathbf{a}_2$ such that the parallelogram generated by $\mathbf{b}_1, \mathbf{b}_2$ has the smallest possible nonzero area. Finally, choose $\mathbf{b}_3 \in G \cap P$ such that the parallelepiped Q generated by $\mathbf{b}_1, \mathbf{b}_2, \mathbf{b}_3$ has the smallest possible nonzero volume. We show that the \mathbf{b}_i have property (6.2). Clearly, these vectors are linearly independent. Given any $\mathbf{a} \in G$ there exist unique real numbers α_i such that

$$\mathbf{a} = \alpha_1 \mathbf{b}_1 + \alpha_2 \mathbf{b}_2 + \alpha_3 \mathbf{b}_3.$$

Let n_i be the largest integer in α_i . Then

$$(6.3) \quad \mathbf{a} - \sum_{i=1}^3 n_i \mathbf{b}_i = \sum_{i=1}^3 \beta_i \mathbf{b}_i = \mathbf{b}$$

with $0 \leq \beta_i < 1$. The vector \mathbf{b} defined by (7.3) is clearly an element of $G \cap Q$. We will show that $\mathbf{b} = \mathbf{0}$.

Suppose $0 < \beta_3 < 1$. Then the volume $V(Q')$ of the parallelepiped Q' generated by $\mathbf{b}_1, \mathbf{b}_2, \mathbf{b}$ is strictly less than the volume $V(Q)$. In fact $V(Q') = \beta_3 V(Q)$, but if $\mathbf{b} \in P$ this is impossible since it contradicts our choice of \mathbf{b}_3 . If $\mathbf{b} \notin P$ we can find integers m_1, m_2 such that $\mathbf{b}' = \mathbf{b} + m_1 \mathbf{a}_1 + m_2 \mathbf{a}_2 \in P$ and the parallelepiped Q'' generated by $\mathbf{b}_1, \mathbf{b}_2, \mathbf{b}'$ has volume $V(Q'') =$

$\beta_3 V(Q) < V(Q)$. This is impossible! Thus $\beta_3 = 0$ and \mathbf{b} lies in the plane spanned by \mathbf{a}_1 and \mathbf{a}_2 . If $0 < \beta_2 < 1$ then the area of the parallelogram generated by \mathbf{b}_1, \mathbf{b} is β_2 times the area of the parallelogram generated by $\mathbf{b}_1, \mathbf{b}_2$, which contradicts the choice of \mathbf{b}_2 if $\mathbf{b} \in P$. If $\mathbf{b} \notin P$ then there is an integer m_1 such that $\mathbf{b}' = \mathbf{b} + m_1 \mathbf{a}_1 \in P$ and the area of the parallelogram generated by $\mathbf{b}_1, \mathbf{b}'$ is β_2 times the area of the parallelogram generated by $\mathbf{b}_1, \mathbf{b}_2$. This is impossible! Thus $\beta_2 = 0$ and $\mathbf{b} = \beta_1 \mathbf{b}_1$. If $0 < \beta_1 < 1$ then \mathbf{b} is closer to $\mathbf{0}$ than is \mathbf{b}_1 . This is impossible, so $\mathbf{b} = \mathbf{0}$. Q.E.D.

Now we return to the idea of the lattice group as a transformation group on R_3 . Suppose the elements $\mathbf{b}_1, \mathbf{b}_2, \mathbf{b}_3$ in G satisfy property (6.2). We call such a triple **basic vectors**. Let $\mathbf{x} \in R_3$. Applying to \mathbf{x} those transformations in G corresponding to $\mathbf{b}_1, \mathbf{b}_2, \mathbf{b}_3, \mathbf{b}_1 + \mathbf{b}_2, \mathbf{b}_1 + \mathbf{b}_3, \mathbf{b}_2 + \mathbf{b}_3$, and $\mathbf{b}_1 + \mathbf{b}_2 + \mathbf{b}_3$, we get a parallelepiped in R_3 called a **primitive cell** or **basic parallelepiped**. By applying all elements of G to \mathbf{x} , i.e., by constructing the G -orbit containing \mathbf{x} , we form a geometrical lattice of points in R_3 . Indeed, it follows from Theorem 2.6 that this lattice is just what we would get by stacking together copies of the primitive cell so that they fill all of R_3 . The lattice points are the vertices of the primitive cells. If the \mathbf{b}_i were linearly independent but did not satisfy (6.2) we could still carry out the above construction and fill R_3 with cells constructed on \mathbf{x} . However, the vertices of these cells would not exhaust the points in the G -orbit containing \mathbf{x} .

We can construct a lattice containing any point \mathbf{x} . Two points lie on the same lattice if and only if they are in the same G -orbit. The totality of all lattices, i.e., all G -orbits, is called the **crystal lattice** or **space lattice**. Ordinarily it is most convenient to discuss lattices based on $\mathbf{x} = \mathbf{0}$.

By suitably eliminating certain faces, edges, and vertices from a primitive cell we can construct a **fundamental domain** for G , i.e., a subset D of R_3 such that any point $\mathbf{x} \in R_3$ lies in the same G -orbit as some $\mathbf{y} \in D$ and no two points in D lie in the same G -orbit. Thus, D consists of exactly one point from each G -orbit of R_3 .

The proof of Theorem 2.6 shows that even though the crystal lattice of G is uniquely determined by G , the primitive cell is not. In fact, there are an infinite number of possible basic vectors \mathbf{b}_i .

Corollary 2.2. Corresponding to any two linearly independent vectors $\mathbf{a}_1, \mathbf{a}_2 \in G$ there exists a primitive cell Q with an edge directed along \mathbf{a}_1 and a face in the plane spanned by \mathbf{a}_1 and \mathbf{a}_2 . (We assume $\mathbf{x} = \mathbf{0}$.)

The primitive cells of G can be characterized as the cells with smallest volume. Let $\mathbf{b}_1, \mathbf{b}_2, \mathbf{b}_3$ be basic vectors with primitive cell Q of volume $V(Q)$ and let $\mathbf{a}_1, \mathbf{a}_2, \mathbf{a}_3$ be three linearly independent vectors in G with cell P .

Theorem 2.7. $V(Q) \leq V(P)$.

Proof. In terms of the standard orthonormal basis vectors $\mathbf{e}_1, \mathbf{e}_2, \mathbf{e}_3$, the \mathbf{a}_i and \mathbf{b}_i can be represented as

$$(6.4) \quad \mathbf{a}_i = \sum_{j=1}^3 a_{ji} \mathbf{e}_j, \quad \mathbf{b}_k = \sum_{j=1}^3 b_{jk} \mathbf{e}_j, \quad i, k = 1, 2, 3,$$

where the 3×3 matrices

$$A = (a_{ij}), \quad B = (b_{kj})$$

are nonsingular. Similarly,

$$(6.5) \quad \mathbf{a}_i = \sum_{k=1}^3 c_{ki} \mathbf{b}_k, \quad i = 1, 2, 3,$$

and the nonsingular matrix

$$C = (c_{ik})$$

has integer matrix elements, since the \mathbf{b}_k are basic vectors. It follows from (6.4) and (6.5) that $A = BC$ in terms of matrix multiplication. Furthermore,

$$(6.6) \quad V(P) = |\mathbf{a}_1 \cdot (\mathbf{a}_2 \times \mathbf{a}_3)| = |\det A|.$$

Thus,

$$(6.7) \quad V(P) = |\det BC| = |\det C| \cdot |\det B| = |\det C| \cdot V(Q),$$

and $|\det C| \geq 1$ since C has integer matrix elements. Q.E.D.

In particular, $V(P)$ is an integral multiple of $V(Q)$.

Corollary 2.3. A primitive cell of G is a cell with minimum nonzero volume. The volumes of any two primitive cells are equal.

Corollary 2.4. If the vectors \mathbf{a}_i in G are related to the basic vectors \mathbf{b}_i by (6.5) then the \mathbf{a}_i are basic vectors if and only if $\det C = \pm 1$.

2.7 Crystallographic Point Groups

Let H be a three-dimensional lattice group and consider the lattice L formed by the action of H on a given point $\mathbf{x} \in R_3$. For convenience we assume $\mathbf{x} = \mathbf{0}$. Since L is a (unbounded) point set in R_3 , it has a complete symmetry group G . We will soon see that G is discrete. Clearly, H is a translation subgroup of G since the elements of H map L onto itself.

Suppose \mathbf{t} is an element of $G \cap T(3)$, i.e., \mathbf{t} is a translation in G . Then $\mathbf{t}\mathbf{0} = \mathbf{b}$ is a lattice point of L . If $\mathbf{b}_1, \mathbf{b}_2, \mathbf{b}_3$ are basic vectors for H there exist unique integers n_i such that

$$\mathbf{b} = n_1 \mathbf{b}_1 + n_2 \mathbf{b}_2 + n_3 \mathbf{b}_3.$$

Since t is a translation it maps any $y \in R_3$ onto $y + n_1\mathbf{b}_1 + n_2\mathbf{b}_2 + n_3\mathbf{b}_3$. Thus, $t \in H$ and $H = G \cap T(3)$.

Now if $g \in G$ then $g\theta = \mathbf{b}$ is a lattice point of L . If $t \in H$ is the lattice translation that maps θ into \mathbf{b} then $t^{-1}g\theta = \theta$, i.e., the transformation $f = t^{-1}g \in G$ leaves the point θ fixed. Thus, every element g of G can be written uniquely in the form $g = tf$, where $t \in H$ and f leaves θ fixed. Denoting by F the subgroup of G fixing θ , we see that $G = HF$ and G is the semidirect product of H and F . In particular the product of two elements t_1f_1 and t_2f_2 in G is given by

$$(7.1) \quad (t_1f_1)(t_2f_2) = t_1(f_1t_2f_1^{-1})(f_1f_2),$$

since $f_1t_2f_1^{-1} \in G \cap T(3) = H$. Furthermore, the elements of G preserve distance and there are only a finite number of lattice points inside any sphere centered at θ , so F must be a finite point group. As a consequence, G is necessarily discrete. Any two three-dimensional lattice groups H_1, H_2 are clearly isomorphic. Thus to compute all complete symmetry groups of lattices up to isomorphism (hence to classify all lattices by symmetry type) it is enough to compute all possible point groups F . An arbitrary symmetry group of L , not necessarily the complete group of symmetries, is an arbitrary subgroup G' of G .

Definition. A subgroup of $E(3)$ which fixes a point x and maps a three-dimensional lattice L containing x into itself is called a **crystallographic point group**. The largest crystallographic point group F at x is called the **holohedry** of L at x .

We have shown that a crystallographic point group is necessarily finite. Furthermore, if x and y are points contained in the same lattice L then the holohedries fixing x and y , respectively, are conjugate subgroups of $E(3)$. The crystallographic point groups are just the subgroups of the holohedries.

Not all point groups are crystallographic point groups. The requirement that a point group leave a lattice invariant is a strong restriction on the elements of the group.

Theorem 2.8. (The crystallographic restriction). Let K be a crystallographic point group. If $g \in K$ is a nontrivial rotation then g is of order two, three, four, or six. If $g = I\mathbf{k}$ is a rotation-inversion in K then the rotation \mathbf{k} is of order one, two, three, four, or six.

Proof. Let $\mathbf{b}_1, \mathbf{b}_2, \mathbf{b}_3$ be basic vectors for the lattice L on which K acts. Writing

$$(7.2) \quad g\mathbf{b}_i = \sum_{j=1}^3 c_{ji}\mathbf{b}_j$$

we see that

$$C = (c_{ij})$$

is the matrix of the transformation \mathbf{g} in the basis $\{\mathbf{b}_i\}$. Recall that the trace of a matrix is invariant under similarity transformations, i.e., the trace of \mathbf{g} is independent of basis. Since the \mathbf{b}_i are basic vectors of L it follows that the c_{ij} are integers, so $\text{tr } C$ is an integer. However, from (1.10), we see that for an orthonormal basis with one basis vector along the axis of rotation, the trace is $\pm(1 + 2 \cos \varphi)$, where φ is the rotation angle corresponding to \mathbf{g} . The minus sign applies to rotation-inversions. Thus,

$$(7.3) \quad \text{tr } C = \pm(1 + 2 \cos \varphi)$$

and the only way this can be an integer is for $\varphi = \pi/2, 3\pi/2, n\pi/3$, with $n = 0, 1, \dots, 5$. (Note that necessarily $|\text{tr } C| \leq 3$.) Q.E.D.

This theorem shows that no point group which contains elements with rotational parts of order five or greater than six can be a crystallographic point group. It follows from our classification of point groups in Sections 2.4 and 2.5 that all but 32 point groups can be eliminated as candidates for crystallographic groups. The possible point groups of the first kind are the cyclic groups C_1, C_2, C_3, C_4, C_6 , the dihedral groups D_2, D_3, D_4, D_6 , the tetrahedral group T , and the octahedral group O . The possible point groups of the second kind are $S_2, S_4, S_6, C_{1h}, C_{2h}, C_{3h}, C_{4h}, C_{6h}, C_{2v}, C_{3v}, C_{4v}, C_{6v}, D_{2h}, D_{3h}, T_h, T_d, D_{4h}, D_{6h}, D_{2d}, D_{3d}$, and O_h . We will show that each member of this list is in fact a symmetry group of some lattice, and we will relate these groups to the study of crystal structure in physics.

We first classify the holohedries (or maximal crystallographic point groups) of lattices.

Definition. Two lattices L, L' are in the same **crystal system** if their holohedries F, F' are conjugate subgroups of $E(3)$.

We know that all lattices of a lattice group H lie in the same crystal system, so it also makes sense to speak of a classification of lattice groups into crystal systems.

The possible holohedries can be obtained from our list of the 32 possible crystallographic point groups. However, the following theorems show that there are at most seven holohedries. Let L be a lattice which for convenience we assume based at $\mathbf{x} = \mathbf{0}$ and let F be its holohedry at \mathbf{x} .

Theorem 2.9. The inversion \mathbf{I} is an element of F .

Proof. If $\mathbf{b}_1, \mathbf{b}_2, \mathbf{b}_3$ are basic vectors for L , the lattice points of L are exactly

the points

$$\mathbf{b} = n_1 \mathbf{b}_1 + n_2 \mathbf{b}_2 + n_3 \mathbf{b}_3, \quad n_1, n_2, n_3 \text{ integers.}$$

It follows from this representation that $-\mathbf{b} \in L$ whenever $\mathbf{b} \in L$. Thus $\mathbf{I} \in F$. Q.E.D.

We conclude that holohedries are necessarily point groups of the second kind containing \mathbf{I} .

Theorem 2.10. If F contains the cyclic subgroup C_n , $n = 3, 4, 6$, then F contains C_{nv} .

Proof. We have to show that if F contains an n -fold rotation axis l then it also contains a reflection plane P in which l lies. (The reflection and C_n generate C_{nv} .) Let $\mathbf{C} \in F$ be a rotation about l with rotation angle $2\pi/n$ and let Q be the plane through $\mathbf{x} = \mathbf{0}$ perpendicular to l . If \mathbf{y} is a lattice point of L not on l then $\mathbf{Cy} - \mathbf{y}$ is a nonzero lattice point lying in Q . Therefore, $Q \cap L$ contains nonzero vectors. Let \mathbf{b}_1 be a nonzero vector of minimum length in $Q \cap L$. According to Theorem 2.6 and its corollary we can embed \mathbf{b}_1 in a system of basic vectors $\mathbf{b}_1, \mathbf{b}_2, \mathbf{b}_3$ for L such that \mathbf{b}_2 lies in Q . In fact we can set $\mathbf{b}_2 = \mathbf{Cb}_1$ (Fig 2.6), for if there is an $\mathbf{a} \in Q \cap L$ in the interior of the parallelogram generated by \mathbf{b}_1 and \mathbf{Cb}_1 , then at least one of the lattice vectors $\mathbf{Cb}_1 - \mathbf{a}, \mathbf{Cb}_1 + \mathbf{b}_1 - \mathbf{a}, \mathbf{b}_1 - \mathbf{a}, \mathbf{a}$ is shorter than \mathbf{b}_1 . This is impossible, so $\mathbf{b}_2 = \mathbf{Cb}_1$. All we know about \mathbf{b}_3 initially is that it is not in Q . We can write it uniquely in the form

$$(7.4) \quad \mathbf{b}_3 = \mathbf{u} + \mathbf{v}$$

where the vector \mathbf{u} points along l and \mathbf{v} lies in Q . (Here, \mathbf{u} and \mathbf{v} are just the projections of \mathbf{b}_3 on l and Q : they are not necessarily lattice vectors.) Since

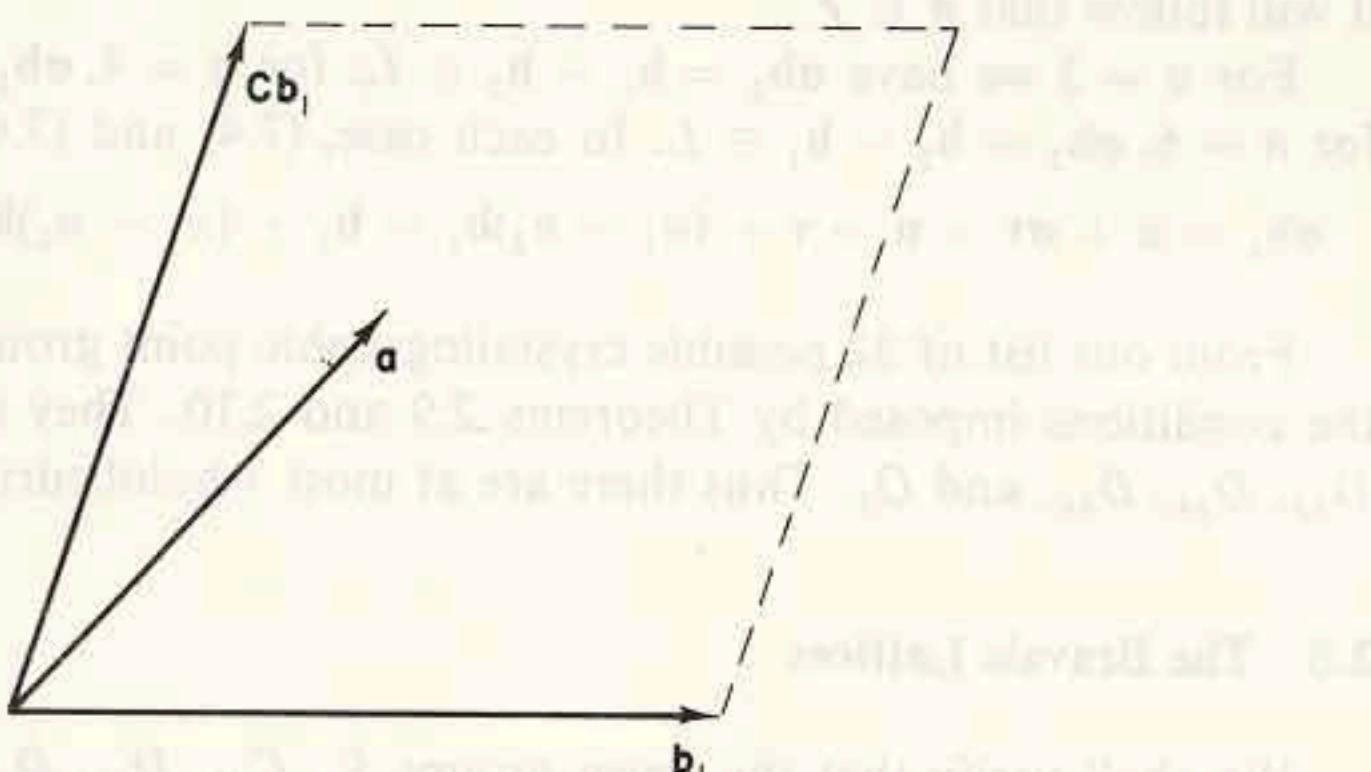


FIGURE 2.6

$\mathbf{C}\mathbf{b}_3 - \mathbf{b}_3 \in L \cap Q$ and $\mathbf{Cu} = \mathbf{u}$, there exist integers n_1, n_2 such that

$$(7.5) \quad \mathbf{C}\mathbf{b}_3 - \mathbf{b}_3 = \mathbf{Cv} - \mathbf{v} = n_1\mathbf{b}_1 + n_2\mathbf{Cb}_1.$$

Multiplying both sides of this expression by \mathbf{C}^{-1} and then subtracting from (7.5) we get

$$\mathbf{Cv} + \mathbf{C}^{-1}\mathbf{v} - 2\mathbf{v} = n_2\mathbf{Cb}_1 - n_1\mathbf{C}^{-1}\mathbf{b}_1 + (n_1 - n_2)\mathbf{b}_1.$$

A little trigonometry yields (Fig. 2.7)

$$\mathbf{Cv} + \mathbf{C}^{-1}\mathbf{v} = 2 \cos(2\pi/n)\mathbf{v},$$

$$\mathbf{Cb}_1 + \mathbf{C}^{-1}\mathbf{b}_1 = 2 \cos(2\pi/n)\mathbf{b}_1.$$

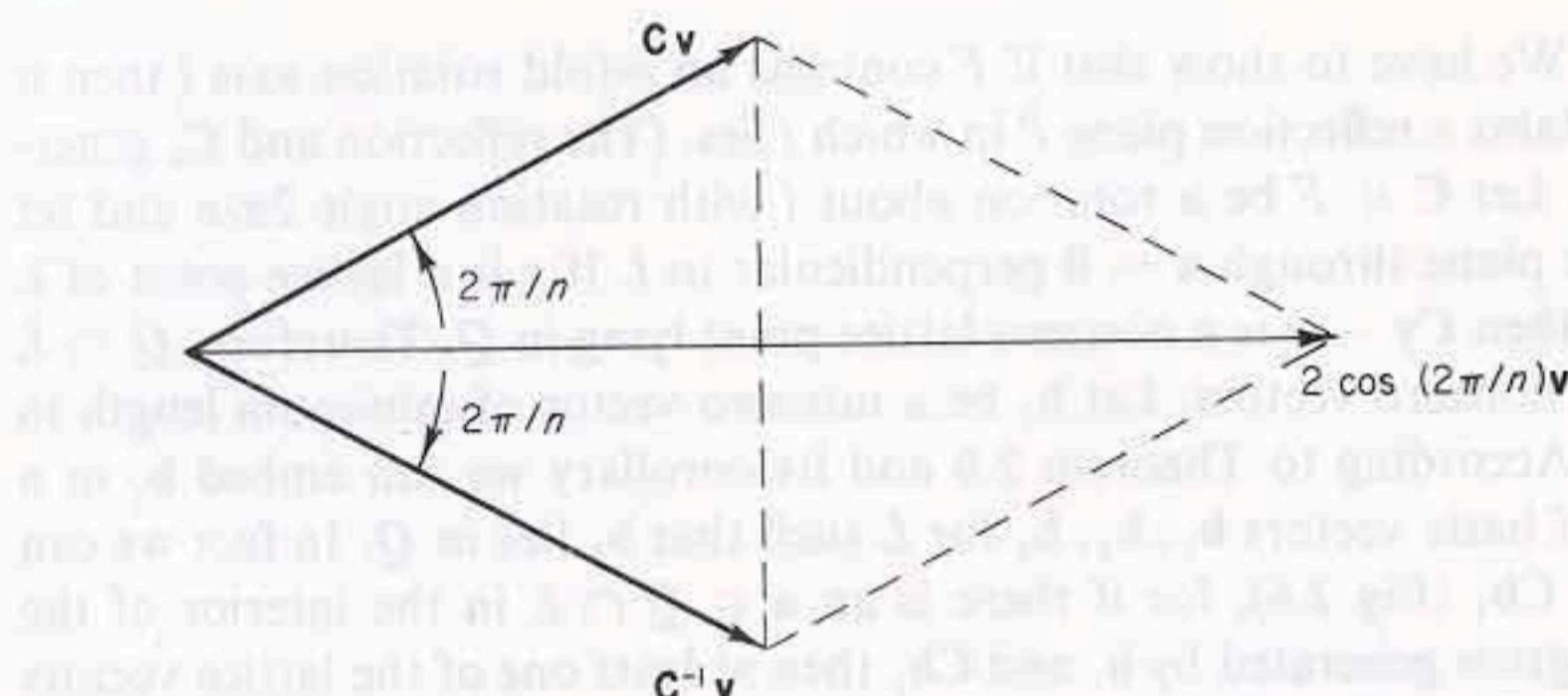


FIGURE 2.7

Thus,

$$(7.6) \quad 2[\cos(2\pi/n) - 1]\mathbf{v} = (n_1 + n_2)\mathbf{b}_2 + [n_1 - n_2 - 2n \cos(2\pi/n)]\mathbf{b}_1.$$

Let σ be the reflection in the plane P containing l and perpendicular to \mathbf{b}_1 . Clearly, $\sigma\mathbf{b}_1 = -\mathbf{b}_1$, $\sigma\mathbf{u} = \mathbf{u}$. If we can show that $\sigma\mathbf{b}_2$ and $\sigma\mathbf{b}_3$ are lattice points it will follow that $\sigma \in F$.

For $n = 3$ we have $\sigma\mathbf{b}_2 = \mathbf{b}_1 + \mathbf{b}_2 \in L$; for $n = 4$, $\sigma\mathbf{b}_2 = \mathbf{b}_2 \in L$; and for $n = 6$, $\sigma\mathbf{b}_2 = \mathbf{b}_2 - \mathbf{b}_1 \in L$. In each case, (7.4) and (7.6) yield

$$\sigma\mathbf{b}_3 = \mathbf{u} + \sigma\mathbf{v} = \mathbf{u} + \mathbf{v} + (n_1 - n_2)\mathbf{b}_1 = \mathbf{b}_3 + (n_1 - n_2)\mathbf{b}_1 \in L. \quad \text{Q.E.D.}$$

From our list of 32 possible crystallographic point groups only 7 satisfy the conditions imposed by Theorems 2.9 and 2.10. They are S_2 , C_{2h} , D_{2h} , D_{3d} , D_{4h} , D_{6h} , and O_h . Thus there are at most 7 holohedries.

2.8 The Bravais Lattices

We shall verify that the seven groups S_2 , C_{2h} , D_{2h} , D_{3d} , D_{4h} , D_{6h} , and O_h are holohedries by explicitly constructing all lattices L for which they are maximal crystallographic point groups. To avoid overly complicated calcula-

tions it is necessary to choose basic vectors for L in a convenient manner. For this, Theorem 2.6 and its corollary will prove useful.

Two lattices (or lattice groups) L_0, L_1 belonging to the same holohedry F are of the same **type** if one of them can be obtained from the other by a continuous lattice deformation L_t , $0 \leq t \leq 1$, in such a way that during the deformation process the holohedry F_t contains F . As we shall see, two lattices belonging to the same holohedry need not have isomorphic complete symmetry groups. However, two lattices belonging to the same type necessarily have isomorphic complete symmetry groups. The seven crystal systems will subdivide into 14 lattice types, the 14 Bravais lattices. Every lattice belongs to exactly one lattice type and this type determines the complete symmetry group of the lattice, up to isomorphism.

Our candidates for holohedries satisfy the subgroup relations given by Fig. 2.8. In particular, $S_2 = \{\mathbf{E}, \mathbf{I}\}$ is contained in all these groups. As we have seen in Theorem 2.9 every lattice admits S_2 as a crystallographic point group.

$$\begin{array}{c} S_2 \subset C_{2h} \subset D_{2h} \subset D_{4h} \subset O_h \\ \cap \quad \cap \\ D_{3d} \subset D_{6h} \end{array}$$

FIGURE 2.8

Except for S_2 , these groups contain an n -fold rotation axis l ($n = 2, 4$, or 6) and a reflection σ_h in the plane P through θ perpendicular to this axis. Let C be a rotation through the angle $2\pi/n$ about l . We will determine the restrictions on a lattice L in order that it admit C and σ_h as symmetries. It is always possible to choose basic vectors $\mathbf{b}_1, \mathbf{b}_2, \mathbf{b}_3$ for L such that \mathbf{b}_1 and \mathbf{b}_2 lie in P . Indeed, if \mathbf{a}_1 and \mathbf{a}_2 are any two lattice points not lying in the same plane containing l then $\mathbf{a}_1 + \sigma_h \mathbf{a}_1$ and $\mathbf{a}_2 + \sigma_h \mathbf{a}_2$ are linearly independent lattice vectors in P . By Corollary 2.2 we can choose \mathbf{b}_1 and \mathbf{b}_2 in P . We write the third basic vector uniquely in the form

$$(8.1) \quad \mathbf{b}_3 = \mathbf{u} + \mathbf{v}$$

where \mathbf{u} lies along l and \mathbf{v} lies in P . Notice that the volume of the cell generated by $\mathbf{b}_1, \mathbf{b}_2, \mathbf{b}_3$ is the same as the volume of the cell generated by $\mathbf{b}_1, \mathbf{b}_2, \mathbf{b}_3'$, where

$$(8.2) \quad \mathbf{b}_3' = \mathbf{b}_3 + m_1 \mathbf{b}_1 + m_2 \mathbf{b}_2$$

and m_1, m_2 are integers. Thus $\mathbf{b}_1, \mathbf{b}_2, \mathbf{b}_3'$ are also basic vectors. We will use this freedom to vary \mathbf{b}_3 in the computations to follow.

Since $\mathbf{C}\mathbf{u} = \mathbf{u}$ it follows that

$$(8.3) \quad \mathbf{C}\mathbf{b}_3 - \mathbf{b}_3 = \mathbf{C}\mathbf{v} - \mathbf{v} = n_1 \mathbf{b}_1 + n_2 \mathbf{b}_2 \in L \cap P.$$

Relation (8.3) will enable us to compute \mathbf{v} , hence to enumerate the possibilities for \mathbf{b}_3 . This enumeration depends on the value of n . If $n = 2$ then $\mathbf{C}\mathbf{v} = -\mathbf{v}$.

Solving for \mathbf{v} in (8.3) and substituting into (8.1), we get

$$(8.4) \quad \mathbf{b}_3 = \mathbf{u} + \frac{1}{2}n_1\mathbf{b}_1 + \frac{1}{2}n_2\mathbf{b}_2.$$

Using the freedom of (8.2) in selecting \mathbf{b}_3 , we can add arbitrary integer multiples of \mathbf{b}_1 and \mathbf{b}_2 to (8.4). Thus, we can choose \mathbf{b}_3 such that $n_1, n_2 = 0, 1$. There are four possibilities:

$$(8.5) \quad \begin{array}{ll} (1) & \mathbf{b}_3 = \mathbf{u}, \\ (2) & \mathbf{b}_3 = \mathbf{u} + \frac{1}{2}\mathbf{b}_1, \\ (3) & \mathbf{b}_3 = \mathbf{u} + \frac{1}{2}\mathbf{b}_2, \\ (4) & \mathbf{b}_3 = \mathbf{u} + \frac{1}{2}\mathbf{b}_1 + \frac{1}{2}\mathbf{b}_2. \end{array}$$

Only in case (1) is \mathbf{b}_3 perpendicular to the plane P . Since \mathbf{b}_1 and \mathbf{b}_2 have not been uniquely specified, these four cases are not all distinct. Under an interchange of \mathbf{b}_1 and \mathbf{b}_2 , (2) and (3) coincide. Furthermore, if \mathbf{b}_1 and \mathbf{b}_2 are replaced by the new basic vectors \mathbf{b}_1 and $\mathbf{b}_1 + \mathbf{b}_2$ then (3) (4) coincide. However, the same lattice cannot have a primitive cell of the form (1) and a primitive cell of the form (2), (3), or (4).

The cases $n = 4, 6$ follow from the proof of Theorem 2.10. It was shown that we can choose \mathbf{b}_1 as the shortest nonzero vector in $P \cap L$ and $\mathbf{b}_2 = \mathbf{C}\mathbf{b}_1$. Then the expression for \mathbf{v} is given by (7.6). If $n = 4$ then

$$\mathbf{b}_3 = \mathbf{u} + \frac{1}{2}(n_2 - n_1)\mathbf{b}_1 - \frac{1}{2}(n_2 + n_1)\mathbf{b}_2.$$

Now $n_2 \pm n_1$ are simultaneously odd or even integers. Thus, addition of integer multiples of \mathbf{b}_1 and \mathbf{b}_2 reduces \mathbf{b}_3 to two normal forms:

$$(8.6) \quad \begin{array}{ll} (1) & \mathbf{b}_3 = \mathbf{u}, \\ (2) & \mathbf{b}_3 = \mathbf{u} + \frac{1}{2}\mathbf{b}_1 + \frac{1}{2}\mathbf{b}_2. \end{array}$$

If $n = 6$, (7.6) yields

$$\mathbf{b}_3 = \mathbf{u} + n_2\mathbf{b}_1 - (n_1 + n_2)\mathbf{b}_2.$$

Addition of $(n_1 + n_2)\mathbf{b}_2 - n_2\mathbf{b}_1$ reduces this to

$$(8.7) \quad \mathbf{b}_3 = \mathbf{u}.$$

Thus, \mathbf{b}_3 can always be chosen perpendicular to \mathbf{b}_1 and $\mathbf{b}_2 = \mathbf{C}\mathbf{b}_1$.

Armed with this information, we examine the holohedries one at a time and determine the lattice types which correspond to them.

The cubic holohedry O_h . Let l be one of the fourfold axes of the group O_h and consider a lattice L with primitive cell corresponding to the choice (1) of (8.6). Thus, the basic vectors are chosen so that (1) they are mutually perpendicular, (2) \mathbf{b}_3 lies on l , and (3) \mathbf{b}_1 and \mathbf{b}_2 have the same (minimal) length. Now O_h has four rotation axes through θ evenly spaced in the plane P spanned by \mathbf{b}_1 and \mathbf{b}_2 , so at least one of these axes l_1 lies between \mathbf{b}_1 and \mathbf{b}_2 (Fig. 2.9). The axis l_1 is at least twofold. Let \mathbf{R} be the rotation through π about l_1 . Then $\mathbf{R}\mathbf{b}_1$ and $\mathbf{R}\mathbf{b}_2$ must lie in $L \cap P$. However, $L \cap P$ is a square grid, so l_1 must be at an angle of $\pi/4$ with both \mathbf{b}_1 and \mathbf{b}_2 . Now l_1 cannot

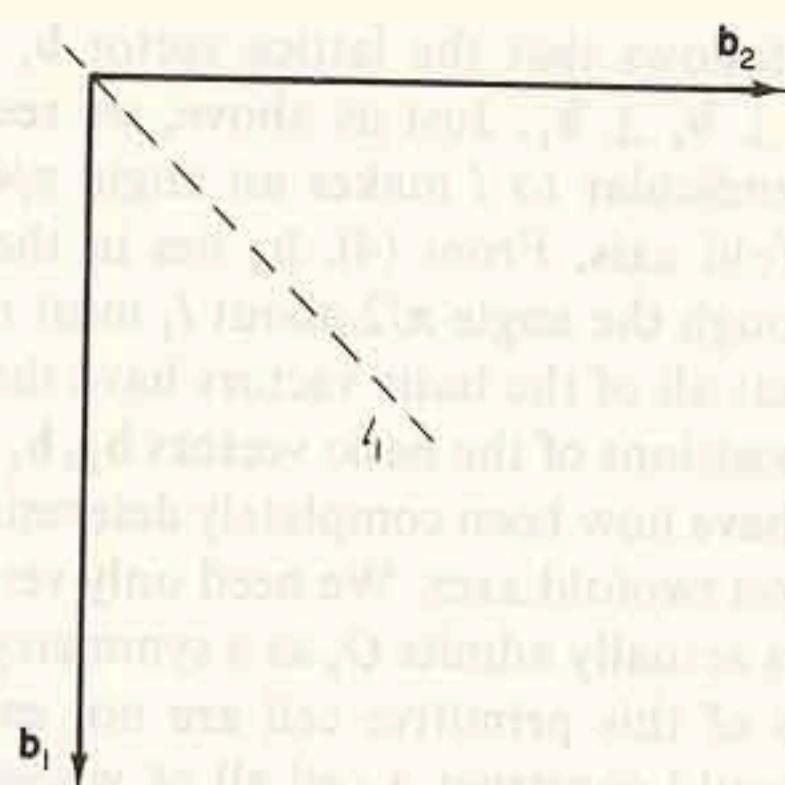
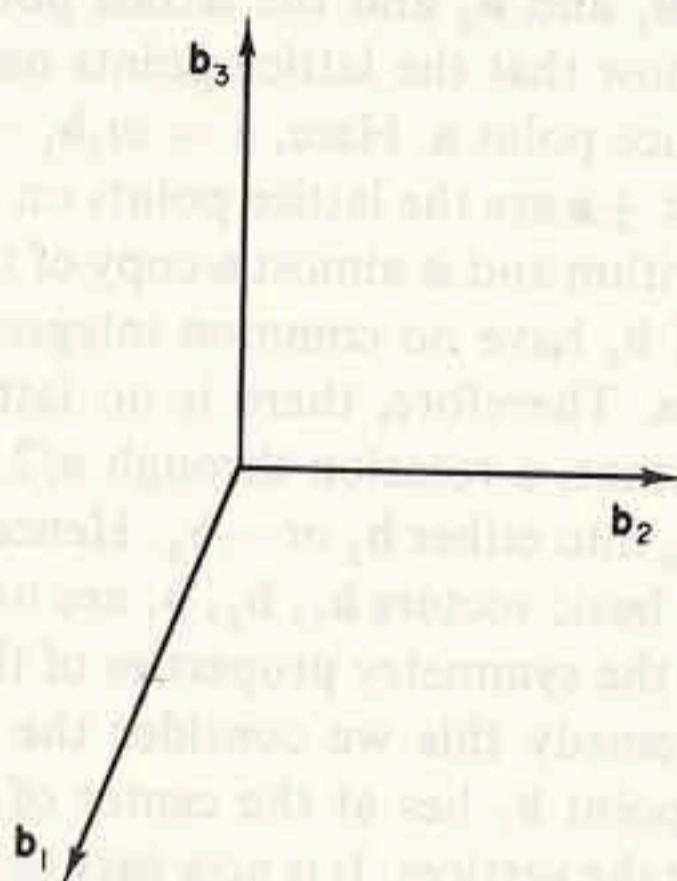


FIGURE 2.9

be a fourfold axis since a rotation of $\pi/2$ about l_1 maps \mathbf{b}_1 and \mathbf{b}_2 into points not in L . Thus, l_1 is a twofold axis and the two fourfold axes in P (which form an angle of $\pi/4$ with l_1) must lie along \mathbf{b}_1 and \mathbf{b}_2 , respectively. A rotation of $\pi/2$ about the axis through \mathbf{b}_2 necessarily maps \mathbf{b}_3 onto \mathbf{b}_1 or $-\mathbf{b}_1$. Therefore, $\|\mathbf{b}_3\| = \|\mathbf{b}_1\|$ and the three basic vectors have the same length. (Fig. 2.10). The primitive cell is a cube Γ_c . It is now clear from the definition of O_h that a lattice of type Γ_c admits O_h as its holohedry. All such lattices can be designated by a single parameter, the length of one side of the primitive cell.

A second possibility is that the primitive cell of the lattice L about the fourfold axis l takes the form (2) in expression (8.6). Thus, (1) $\mathbf{b}_1 \perp \mathbf{b}_2$, (2) the basic vectors $\mathbf{b}_1, \mathbf{b}_2$ are perpendicular to l and have minimal length in the set of such lattice vectors, (3) $\|\mathbf{b}_1\| = \|\mathbf{b}_2\|$, and (4) $\mathbf{b}_3 = \mathbf{u} + \frac{1}{2}\mathbf{b}_1 + \frac{1}{2}\mathbf{b}_2$,

FIGURE 2.10. Here, $\mathbf{b}_1 \perp \mathbf{b}_2 \perp \mathbf{b}_3 \perp \mathbf{b}_1$; $\|\mathbf{b}_1\| = \|\mathbf{b}_2\| = \|\mathbf{b}_3\|$.

where \mathbf{u} lies along l . It follows that the lattice vector $\mathbf{b}_4 = 2\mathbf{b}_3 - \mathbf{b}_1 - \mathbf{b}_2$ lies on l . Thus, $\mathbf{b}_1 \perp \mathbf{b}_2 \perp \mathbf{b}_4 \perp \mathbf{b}_1$. Just as above, we see that the twofold or fourfold axis l_1 perpendicular to l makes an angle $\pi/4$ with \mathbf{b}_1 and \mathbf{b}_2 .

Suppose l_1 is a fourfold axis. From (4), \mathbf{b}_3 lies in the plane through l and l_1 , so a rotation through the angle $\pi/2$ about l_1 must map \mathbf{b}_3 into either \mathbf{b}_1 or \mathbf{b}_2 . We conclude that all of the basic vectors have the same length and $\|\mathbf{b}_4\| = \sqrt{2}\|\mathbf{b}_1\|$. The positions of the basic vectors $\mathbf{b}_1, \mathbf{b}_2, \mathbf{b}_3$ and the orientation of the axes of O_h have now been completely determined. In particular, the vectors \mathbf{b}_1 and \mathbf{b}_2 lie on twofold axes. We need only verify that the lattice L with these basic vectors actually admits O_h as a symmetry group. However, the symmetry properties of this primitive cell are not easy to visualize. It would be helpful if we could construct a cell all of whose vertices were on fourfold axes. This can be achieved by using the lattice vectors $\mathbf{b}_1 + \mathbf{b}_2$, $\mathbf{b}_1 - \mathbf{b}_2$, and \mathbf{b}_4 to generate a cube Γ_c^f . (Note that $\mathbf{b}_1 + \mathbf{b}_2$ lies on l_1 and $\mathbf{b}_1 - \mathbf{b}_2$ lies on another fourfold axis.) The lattice points $\mathbf{b}_3, \mathbf{b}_3 - \mathbf{b}_2, \mathbf{b}_3 + \mathbf{b}_1$, and $\mathbf{b}_3 + \mathbf{b}_1 - \mathbf{b}_2$ are the midpoints of the four vertical faces of Γ_c^f , \mathbf{b}_1 is the midpoint of the bottom face, and $\mathbf{b}_4 + \mathbf{b}_1$ is the midpoint of the top face. All of the remaining lattice points in Γ_c^f lie at the vertices. It is now easy to check that a lattice built from cells of type Γ_c^f admits O_h as a symmetry group. Lattices with type Γ_c^f symmetry are called **face-centered cubic**. The cell Γ_c^f is not primitive since its volume is four times that of a primitive cell. However, in practice the face-centered cubic cell is often preferable to a primitive cell since it exhibits O_h symmetry in a very explicit form. All lattices of type Γ_c^f can be described by a single parameter, the length of one side of the face-centered cube.

The only remaining possibility is that l_1 is a twofold axis. In this case fourfold axes lie along \mathbf{b}_1 and \mathbf{b}_2 and the lattice point $\mathbf{b}_4 = 2\mathbf{b}_3 - \mathbf{b}_1 - \mathbf{b}_2$ lies on l . It is easy to show that the lattice points on l consist of all integer multiples of a single lattice point \mathbf{a} . Here, $\mathbf{a} = m_1\mathbf{b}_1 + m_2\mathbf{b}_2 + m_3\mathbf{b}_3$ is characterized by the fact that $\pm\mathbf{a}$ are the lattice points on l closest to $\mathbf{0}$. The proof uses the Euclidean algorithm and is almost a copy of the proof of Lemma 2.2. Since the coefficients of \mathbf{b}_4 have no common integer divisor other than ± 1 it follows that $\mathbf{b}_4 = \pm\mathbf{a}$. Therefore, there is no lattice point on l between $\mathbf{0}$ and \mathbf{b}_4 . As a consequence, a rotation through $\pi/2$ radians about the fourfold axis \mathbf{b}_1 must map \mathbf{b}_4 into either \mathbf{b}_2 or $-\mathbf{b}_2$. Hence, $\|\mathbf{b}_1\| = \|\mathbf{b}_2\| = \|\mathbf{b}_4\|$ and the positions of the basic vectors $\mathbf{b}_1, \mathbf{b}_2, \mathbf{b}_3$ are uniquely determined. Just as in the previous case, the symmetry properties of the primitive cell are not easy to visualize. To remedy this we consider the cube Γ_c^v generated by $\mathbf{b}_1, \mathbf{b}_2, \mathbf{b}_4$. The lattice point \mathbf{b}_3 lies at the center of Γ_c^v and the remaining lattice points in Γ_c^v lie at the vertices. It is now easy to check that a lattice constructed from type $-\Gamma_c^v$ cells actually admits O_h as a symmetry group. Such lattices are called **body-centered cubic**. The volume of a Γ_c^v cell is twice that

of a primitive cell. All lattices of type Γ_c^v can be described uniquely in terms of the length of one side of a body-centered cell.

We have shown that the crystal system with cubic holohedry O_h divides into three lattice types: primitive Γ_c , face-centered Γ_c^f , and body-centered Γ_c^v .

The hexagonal holohedry D_{6h} . Let l be the sixfold axis of D_{6h} and consider a lattice L admitting D_{6h} as a symmetry group. Since D_{6h} is not a proper subgroup of any possible holohedry, it must be the holohedry of L . According to (8.7) we can find vectors $\mathbf{b}_1, \mathbf{b}_2, \mathbf{b}_3$ for L such that (1) the angle between \mathbf{b}_1 and \mathbf{b}_2 is $\pi/3$, (2) $\mathbf{b}_1 \perp \mathbf{b}_3 \perp \mathbf{b}_2$, and (3) \mathbf{b}_1 and \mathbf{b}_2 have the same (minimal) length and lie in the plane P through Θ and perpendicular to l . Conversely, it is straightforward to show that a lattice L with basic vectors satisfying (1)–(3) actually admits D_{6h} as a symmetry group. The primitive cell just constructed is denoted Γ_h . Lattices of type Γ_h are uniquely determined by two parameters: $\|\mathbf{b}_1\|$ and $\|\mathbf{b}_3\|$.

The tetragonal holohedry D_{4h} . Let l be the fourfold axis of D_{4h} and L a lattice with primitive cell corresponding to choice (1) of (8.6). Then (1) $\mathbf{b}_1 \perp \mathbf{b}_2 \perp \mathbf{b}_3 \perp \mathbf{b}_1$ and (2) \mathbf{b}_1 and \mathbf{b}_2 have the same (minimal) length both lying in the plane P through Θ perpendicular to l . Conversely, it is easy to show that any lattice with primitive cell satisfying (1) and (2) admits D_{4h} as a symmetry group. In order that D_{4h} qualify as the holohedry of L it is necessary to require $\|\mathbf{b}_1\| \neq \|\mathbf{b}_3\|$. Otherwise L would have O_h as holohedry. The primitive cell just constructed is denoted Γ_q . Lattices of type Γ_q are determined by the two parameters $\|\mathbf{b}_1\|$ and $\|\mathbf{b}_3\|$.

Now suppose the primitive cell of L about the fourfold axis l takes the form (2) of expression (8.6). Then (1) \mathbf{b}_1 and \mathbf{b}_2 are vectors of minimal length in the plane P perpendicular to l and passing through Θ , (2) $\mathbf{b}_1 \perp \mathbf{b}_2$, (3) $\|\mathbf{b}_1\| = \|\mathbf{b}_2\|$, and (4) $\mathbf{b}_3 = \mathbf{u} + \frac{1}{2}\mathbf{b}_1 + \frac{1}{2}\mathbf{b}_2$, where \mathbf{u} lies on l . Clearly, the lattice vector $\mathbf{b}_4 = 2\mathbf{u} = 2\mathbf{b}_3 - \mathbf{b}_1 - \mathbf{b}_2$ also lies on l , and there is no lattice vector on l between \mathbf{b}_4 and Θ . The vectors $\mathbf{b}_1, \mathbf{b}_2, \mathbf{b}_4$ are mutually orthogonal. The group D_{4h} has four twofold axes lying in P and it is obvious that one axis lies along \mathbf{b}_1 , one axis lies along \mathbf{b}_2 , and a third axis makes an angle of $\pi/4$ with \mathbf{b}_1 and \mathbf{b}_2 . Let Γ_q^v be the rectangular parallelepiped (box) generated by $\mathbf{b}_1, \mathbf{b}_2, \mathbf{b}_4$. The lattice point \mathbf{b}_3 lies at the center of Γ_q^v but all other lattice points are located at the vertices. Clearly, a lattice constructed from Γ_q^v cells admits D_{4h} as a symmetry group. However, D_{4h} is the holohedry only if $\|\mathbf{b}_4\| \neq \|\mathbf{b}_1\|$, since otherwise the holohedry would be O_h . Note that Γ_q^v has twice the volume of a primitive cell. A lattice of type Γ_q^v is called **body-centered**. All lattices of type Γ_q^v can be described by the two parameters $\|\mathbf{b}_1\|$ and $\|\mathbf{b}_4\|$.

We have shown that the crystal system with tetragonal holohedry contains two lattice types: primitive Γ_q and body-centered Γ_q^v .

The rhombohedral holohedry D_{3d} . Let l be the threefold axis of D_{3d} and let P be the plane through l perpendicular to l . Suppose C is a rotation through the angle $2\pi/3$ about l . Then we can choose basic vectors $\mathbf{b}_1, \mathbf{b}_2, \mathbf{b}_3$ (Fig. 2.11) for L such that \mathbf{b}_1 has minimal nonzero length in $L \cap P$ and $\mathbf{b}_2 = C\mathbf{b}_1$.

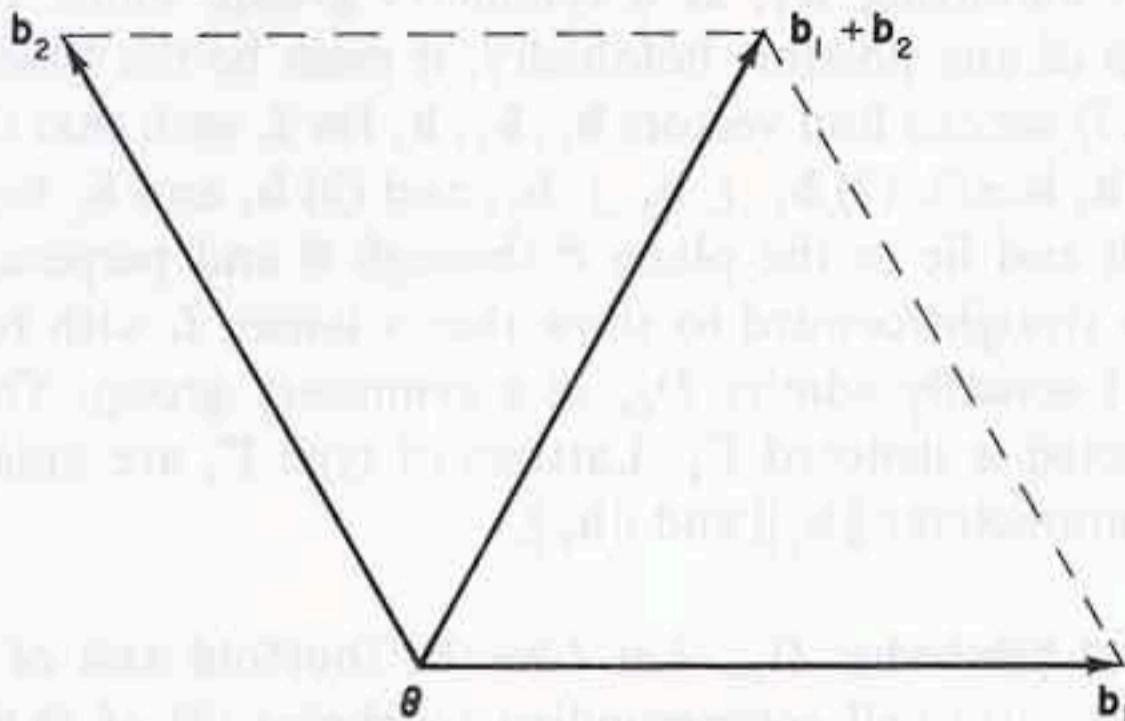


FIGURE 2.11

Write $\mathbf{b}_3 = \mathbf{u} + \mathbf{v}$, where \mathbf{u} lies along l and \mathbf{v} lies in P . Let $S \in D_{3d}$ be the rotation through the angle $\pi/3$ about l followed by a reflection in P . Clearly, $S\mathbf{u} = -\mathbf{u}$, $S\mathbf{b}_1 = \mathbf{b}_1 + \mathbf{b}_2$, and $S\mathbf{b}_2 = -\mathbf{b}_1$. In particular,

$$(8.8) \quad S\mathbf{b}_3 + \mathbf{b}_3 = S\mathbf{v} + \mathbf{v} = n_1\mathbf{b}_1 + n_2\mathbf{b}_2 \in L \cap P,$$

where n_1, n_2 are integers. Multiplying both sides of (8.8) by S^{-1} , we obtain

$$(8.9) \quad \mathbf{v} + S^{-1}\mathbf{v} = (n_2 - n_1)\mathbf{b}_1 + n_2\mathbf{b}_2.$$

Addition of (8.8) and (8.9) yields

$$S\mathbf{v} + S^{-1}\mathbf{v} + 2\mathbf{v} = (n_1 + n_2)\mathbf{b}_1 + (2n_2 - n_1)\mathbf{b}_2.$$

A computation exactly like that following (7.5) shows that the left-hand side is $3\mathbf{v}$. Thus,

$$(8.10) \quad \mathbf{b}_3 = \mathbf{u} + \frac{1}{3}(n_1 + n_2)\mathbf{b}_1 + \frac{1}{3}(2n_2 - n_1)\mathbf{b}_2.$$

As usual, we can subtract arbitrary integer multiples of \mathbf{b}_1 and \mathbf{b}_2 from \mathbf{b}_3 and still maintain a primitive cell. There are only three distinct possibilities:

(8.11)

$$(1) \quad \mathbf{b}_3 = \mathbf{u}, \quad (2) \quad \mathbf{b}_3 = \mathbf{u} + \frac{1}{3}(\mathbf{b}_1 - \mathbf{b}_2), \quad (3) \quad \mathbf{b}_3 = \mathbf{u} - \frac{1}{3}(\mathbf{b}_1 - \mathbf{b}_2).$$

Case (1) is ruled out. For, if $\mathbf{b}_3 = \mathbf{u}$ it is easy to see that the primitive cell generated by $\mathbf{b}_1, \mathbf{b}_1 + \mathbf{b}_2, \mathbf{b}_3$ is just Γ_h , so L has holohedry D_{6h} . Furthermore, cases (2) and (3) are really the same since the lattice does not furnish us with

an orientation with which to tell \mathbf{b}_1 and \mathbf{b}_2 apart. We choose (2) as our normal form. Note that the lattice point $3\mathbf{u} = 3\mathbf{b}_3 - \mathbf{b}_1 + \mathbf{b}_2$ lies on l and there are no lattice points on l between $3\mathbf{u}$ and $\mathbf{0}$. It is left to the reader to verify that the three twofold axes of D_{3d} must lie along \mathbf{b}_1 , $\mathbf{b}_1 + \mathbf{b}_2$, and \mathbf{b}_2 , respectively, and the three vertical reflection planes bisect the angles between adjacent twofold axes. The primitive cell generated by \mathbf{b}_1 , \mathbf{b}_2 , \mathbf{b}_3 is denoted Γ_{rh} . It is now straightforward to check that a lattice of type Γ_{rh} does indeed have D_{3d} as its holohedry. All lattices of type Γ_{rh} are uniquely described by the two parameters $\|\mathbf{b}_1\|$ and $\|\mathbf{u}\|$.

The orthorhombic holohedry D_{2h} . Let l be a twofold axis of D_{2h} . Using Corollary 2.2, we choose a primitive cell for L such that \mathbf{b}_1 , \mathbf{b}_2 lie in the plane P through $\mathbf{0}$, perpendicular to l . Assume the lattice corresponds to choice (1) of (8.5) and recall that D_{2h} has two perpendicular twofold axes l_1 , l_2 in the plane P and two vertical reflection planes each containing l with one of the l_i . It is an elementary computation to show that there are only two possibilities: either (1) the l_i lie along \mathbf{b}_1 and \mathbf{b}_2 , or (2) $\|\mathbf{b}_1\| = \|\mathbf{b}_2\|$ and the l_i are the two perpendicular bisectors of the angles between the vectors \mathbf{b}_1 , \mathbf{b}_2 in P . In the first case the \mathbf{b}_i are mutually orthogonal and generate a primitive right parallelepiped Γ_o . In order that D_{2h} be the holohedry of a lattice constructed from type Γ_o cells it is necessary and sufficient that the lengths of no two sides of the primitive cell be equal. The type- Γ_o lattices are determined by three parameters.

Since $\|\mathbf{b}_1\| = \|\mathbf{b}_2\|$ in case (2), it is clear that the lattice vectors $\mathbf{b}_1 \pm \mathbf{b}_2$ and \mathbf{b}_3 generate a right parallelepiped Γ_o^b . The lattice point \mathbf{b}_1 is the midpoint of the base and $\mathbf{b}_3 + \mathbf{b}_1$ is the midpoint of the top of Γ_o^b . The only remaining lattice points in this cell are the vertices. For this reason Γ_o^b is called **base-centered**. The volume of Γ_o^b is twice the volume of a primitive cell. Clearly, a type- Γ_o^b lattice admits D_{2h} as a symmetry group, but D_{2h} is the holohedry of the lattice only if the angle between \mathbf{b}_1 and \mathbf{b}_2 is not $\pi/2$ or $\pi/3$. The type- Γ_o^b lattices are determined by three parameters: $\|\mathbf{b}_1\|$, $\|\mathbf{b}_3\|$, and the angle between \mathbf{b}_1 and \mathbf{b}_2 .

As remarked in the discussion following expressions (8.5), the choices (2)–(4) for \mathbf{b}_3 are not distinct. For normalization purposes we choose $\mathbf{b}_3 = \mathbf{u} + \frac{1}{2}\mathbf{b}_1 + \frac{1}{2}\mathbf{b}_2$. Again there are two possibilities: either (1) the mutually orthogonal twofold axes l_1 , l_2 in P lie along \mathbf{b}_1 and \mathbf{b}_2 , or (2) the l_i are bisectors of the angles between \mathbf{b}_1 , \mathbf{b}_2 , and $\|\mathbf{b}_1\| = \|\mathbf{b}_2\|$. In case (1) we see that \mathbf{b}_1 , \mathbf{b}_2 , and $2\mathbf{u} = 2\mathbf{b}_3 - \mathbf{b}_1 - \mathbf{b}_2$ are mutually orthogonal lattice vectors which generate a right parallelepiped Γ_o^v . The only lattice point in Γ_o^v other than the vertices is \mathbf{b}_3 , the midpoint of Γ_o^v . The cell Γ_o^v is called **body-centered**. It is now easy to check that a lattice constructed from type- Γ_o^v cells admits D_{2h} as a symmetry group. However, D_{2h} is a holohedry of such a lattice only if $\|\mathbf{b}_1\| \neq \|\mathbf{b}_2\|$, since otherwise D_{4h} would be a symmetry of the lattice. The

volume of Γ_o^v is twice the volume of a primitive cell. The type- Γ_o^v lattices can be described by three parameters, the dimensions of the body-centered cell.

Corresponding to possibility (2) above we see that $\mathbf{b}_1 + \mathbf{b}_2$, $\mathbf{b}_1 - \mathbf{b}_2$, and $2\mathbf{u} = 2\mathbf{b}_3 - \mathbf{b}_1 - \mathbf{b}_2$ are mutually orthogonal and generate a right parallelepiped Γ_o^f . This cell clearly contains lattice points only at its vertices and at the midpoints of each of its six faces. For obvious reasons Γ_o^f is called **face-centered**. Type Γ_o^f lattices clearly admit D_{2h} as a symmetry group. However, D_{2h} is the holohedry of such lattices only if the base of Γ_o^f is not square. The volume of the face-centered cell is four times the volume of a primitive cell. The possible type Γ_o^f lattices are determined by three parameters, the dimensions of Γ_o^f .

The crystal system with holohedry D_{2h} thus contains four lattice types: primitive Γ_o , base-centered Γ_o^b , body-centered Γ_o^v , and face-centered Γ_o^f .

The monoclinic holohedry C_{2h} . Let l be the twofold axis of C_{2h} . We can choose basic vectors for the lattice L such that $\mathbf{b}_1, \mathbf{b}_2$ are vectors of minimal length in the plane P perpendicular to l and, by (8.5), we can assume that either $\mathbf{b}_3 = \mathbf{u}$ or $\mathbf{b}_3 = \mathbf{u} + \frac{1}{2}\mathbf{b}_2$. If $\mathbf{b}_3 = \mathbf{u}$ then \mathbf{b}_3 is perpendicular to $\mathbf{b}_1, \mathbf{b}_2$ and the basic vectors generate a primitive cell Γ_m . It is obvious that type Γ_m lattices admit C_{2h} as a symmetry group. However, C_{2h} is a holohedry only if the Γ_m cell does not coincide with Γ_q , Γ_{rh} , Γ_h , or Γ_c . The type- Γ_m lattices are determined by four parameters: $\|\mathbf{b}_1\|, \|\mathbf{b}_2\|, \|\mathbf{b}_3\|$, and the angle between \mathbf{b}_1 and \mathbf{b}_2 .

If $\mathbf{b}_3 = \mathbf{u} + \frac{1}{2}\mathbf{b}_2$ then $\mathbf{b}_4 = 2\mathbf{b}_3 - \mathbf{b}_2$ lies on l . The lattice vectors $\mathbf{b}_1, \mathbf{b}_2, \mathbf{b}_4$ generate the **base-centered** cell Γ_m^b . This cell contains only the lattice point \mathbf{b}_3 as the center of one face and $\mathbf{b}_3 + \mathbf{b}_1$ as the center of the opposite face, in addition to the vertices. A type Γ_m^b lattice admits C_{2h} as a symmetry group, but C_{2h} is the holohedry of such a lattice only if \mathbf{b}_1 is not perpendicular to \mathbf{b}_2 or $\mathbf{b}_1 + \mathbf{b}_2$. The type Γ_m^b lattices can be determined by four parameters: $\|\mathbf{b}_1\|, \|\mathbf{b}_2\|, \|\mathbf{b}_4\|$, and the angle between \mathbf{b}_1 and \mathbf{b}_2 . (If we had chosen \mathbf{b}_3 in the form $\mathbf{b}_3 = \mathbf{u} + \frac{1}{2}\mathbf{b}_1 + \frac{1}{2}\mathbf{b}_2$ we would have been led naturally to a body-centered cell. The choice of Γ_m^b rather than a body-centered cell to designate this lattice type is a matter of custom rather than logical necessity.)

We have shown that the monoclinic crystal system contains two lattice types: primitive Γ_m and base-centered Γ_m^b .

The triclinic holohedry S_2 . Since every lattice admits S_2 as a symmetry group, S_2 is the holohedry for all lattices which do not fall into one of the thirteen lattice types classified above. We can uniquely define basic vectors for such a lattice by requiring $\mathbf{b}_1, \mathbf{b}_2, \mathbf{b}_3$, not all lying in the same plane, to have minimal nonzero distance from $\mathbf{0}$. (A precise definition of the \mathbf{b}_i to obtain uniqueness is a matter of taste.) The basic vectors generate a primitive

lattice Γ_t . The lattices of type Γ_t can be designated by six parameters: the lengths of the three basic vectors and the three angles between pairs of basic vectors.

In conclusion, we have verified our list of 7 holohedries or crystal systems and have shown that there exist 14 lattice types (Bravais lattices).

The crystallographic point groups are just the possible subgroups of the 7 holohedries. It was shown in Section 2.7 that there are at most 32 such groups. Furthermore, it is easy to check that each of the 32 groups is a subgroup of at least one holohedry. Therefore, there are exactly 32 crystallographic point groups. Crystallographers say that there are 32 **crystal classes**.

TABLE 2.2 THE BRAVAIS LATTICES

Bravais lattice	Crystal classes	Basic vectors $\mathbf{b}_1, \mathbf{b}_2, \mathbf{b}_3$
1. Triclinic S_2 Γ_t primitive	$S_2, C_1 = [\mathbf{E}]$	Arbitrary
2. Monoclinic C_{2h} Γ_m primitive Γ_m^b base-centered	C_{2h}, C_2, C_{1h}	$\mathbf{b}_2 \perp \mathbf{b}_3 \perp \mathbf{b}_1$ $\mathbf{b}_1 \perp \mathbf{b}_2 \perp (2\mathbf{b}_3 - \mathbf{b}_2) \perp \mathbf{b}_1$
3. Orthorhombic D_{2h} Γ_o primitive Γ_o^b base-centered Γ_o^v body-centered Γ_o^f face-centered	D_{2h}, D_2, C_{2v}	$\mathbf{b}_1 \perp \mathbf{b}_2 \perp \mathbf{b}_3 \perp \mathbf{b}_1$ $\mathbf{b}_3 \perp (\mathbf{b}_1 + \mathbf{b}_2) \perp (\mathbf{b}_1 - \mathbf{b}_3) \perp \mathbf{b}_3$, $\ \mathbf{b}_1\ = \ \mathbf{b}_2\ $ $\mathbf{b}_1 \perp \mathbf{b}_2 \perp (2\mathbf{b}_3 - \mathbf{b}_1 - \mathbf{b}_2) \perp \mathbf{b}_1$, $\ \mathbf{b}_1\ = \ \mathbf{b}_2\ $ $(\mathbf{b}_1 + \mathbf{b}_2) \perp (\mathbf{b}_1 - \mathbf{b}_2)$ $\perp (2\mathbf{b}_3 - \mathbf{b}_1 - \mathbf{b}_2) \perp (\mathbf{b}_1 + \mathbf{b}_2)$
4. Tetragonal D_{4h} Γ_q primitive Γ_q^v body-centered	$D_{4h}, D_4, C_{4v}, C_{4h}$, C_4, D_{2d}, S_4	$\mathbf{b}_1 \perp \mathbf{b}_2 \perp \mathbf{b}_3 \perp \mathbf{b}_1, \ \mathbf{b}_1\ = \ \mathbf{b}_2\ $ $\mathbf{b}_1 \perp (2\mathbf{b}_3 - \mathbf{b}_1 - \mathbf{b}_2) \perp \mathbf{b}_2 \perp \mathbf{b}_1$, $\ \mathbf{b}_1\ = \ \mathbf{b}_2\ $
5. Rhombohedral D_{3d} Γ_{rh} primitive	D_{3d}, D_3, C_{3v} , S_6, C_3	$\mathbf{b}_1 \perp (2\mathbf{b}_3 - \mathbf{b}_1 + \mathbf{b}_2) \perp \mathbf{b}_2$, $\ \mathbf{b}_1\ = \ \mathbf{b}_2\ , \angle \mathbf{b}_1 \mathbf{b}_2 = 2\pi/3$
6. Hexagonal D_{6h} Γ_h primitive	D_{6h}, C_{6h}, C_{6v} , D_{3h}, C_{3h}, C_6, D_6	$\mathbf{b}_1 \perp \mathbf{b}_3 \perp \mathbf{b}_2, \ \mathbf{b}_1\ = \ \mathbf{b}_2\ $, $\angle \mathbf{b}_1 \mathbf{b}_2 = \pi/3$
7. Cubic O_h Γ_c primitive Γ_c^v body-centered Γ_c^f face-centered	O_h, O, T_d, T_h, T	$\mathbf{b}_1 \perp \mathbf{b}_2 \perp \mathbf{b}_3 \perp \mathbf{b}_1$, $\ \mathbf{b}_1\ = \ \mathbf{b}_2\ = \ \mathbf{b}_3\ $ $\mathbf{b}_1 \perp \mathbf{b}_2 \perp \mathbf{b}_4 \perp \mathbf{b}_1$, $\ \mathbf{b}_1\ = \ \mathbf{b}_2\ = \ \mathbf{b}_4\ $, $\mathbf{b}_4 = 2\mathbf{b}_3 - \mathbf{b}_1 - \mathbf{b}_2$ $\mathbf{b}_1 \perp \mathbf{b}_2 \perp \mathbf{b}_4 \perp \mathbf{b}_1$, $\ \mathbf{b}_1\ = \ \mathbf{b}_2\ = (1/\sqrt{2}) \ \mathbf{b}_4\ $, $\mathbf{b}_4 = 2\mathbf{b}_3 - \mathbf{b}_1$

A crystal class or point group K is said to belong to a crystal system with holohedry F if F is the smallest holohedry containing K . The distribution of crystal classes among the crystal systems is indicated in Table 2.2.

2.9 Crystal Structure

In this section the use of the term “crystal,” introduced earlier, will be given a physical justification.

First we justify our restriction to discrete (even finite) point groups to describe the symmetries of a body S of finite extent. If we believe the atomic theory we can assume S is made up of n atoms. (For the purposes of this discussion think of an atom as a tiny billiard ball.) Every Euclidean symmetry of S must then induce a permutation of these n atoms. If the atoms do not all lie in a single plane then the symmetry \mathbf{g} of S is uniquely determined by the permutation it induces. Since there are at most $n!$ permutations of the n atoms, the complete symmetry group G of S must be finite with order dividing $n!$.

If the atoms of S lie in a plane P but not along a single line then a symmetry \mathbf{g} is determined by the permutation it induces, up to a possible reflection in P . The order of the complete symmetry group G of S is a divisor of $2n!$. The order of G is twice the order of the plane symmetry group obtained by considering S as a subset of R_2 .

If the atoms of S lie on a single axis l then the symmetry group will no longer be discrete. Indeed, if S consists of a single atom the complete symmetry group is the orthogonal group $O(3)$. If S contains more than one atom strung along l then S admits the nondiscrete symmetry group $C_{\infty v}$ consisting of all rotations about l and reflections in all planes passing through l . If in addition S admits a reflection σ in a plane P perpendicular to l then $D_{\infty h} = C_{\infty v} \times \{\mathbf{E}, \sigma\}$ is the complete symmetry group of S . If S does not admit a reflection σ then $C_{\infty v}$ is the complete symmetry group. This concludes our catalog of possible point groups.

Next we discuss the relationship between physical crystals and the lattice groups and crystallographic point groups introduced in the preceding sections. We first assume that the crystal occupies all space. (In this way we can avoid the consideration of the crystal boundary.) Roughly speaking, we can think of a crystal as formed by stacking together identical copies of a unit cell C so as to fill all space. The unit cell contains some given distribution of atoms, all atoms vibrating about equilibrium points in the crystal.

Two points \mathbf{x} and \mathbf{y} in a crystal are said to be **equivalent** if all of the (time-averaged) physical properties of the crystal are identical at \mathbf{x} and \mathbf{y} . In other words \mathbf{x} and \mathbf{y} are equivalent points if there is no operational way of distin-

guishing between them. The crystal as viewed by an observer at \mathbf{x} appears identical to that as viewed by an observer at \mathbf{y} . Only time-averaged properties are considered so as to avoid asymmetries due to the fluctuations of the atoms alone. (We can think of the atoms as frozen at their points of equilibrium.) It is clear that the point \mathbf{x} is equivalent to at least all points of the form $\mathbf{x} + n_1\mathbf{b}_1 + n_2\mathbf{b}_2 + n_3\mathbf{b}_3$, where n_1, n_2, n_3 are arbitrary integers and $\mathbf{b}_1, \mathbf{b}_2, \mathbf{b}_3$ are the vectors generating C .

We define the complete symmetry group of a crystal as the subgroup of $E(3)$ consisting of those Euclidean motions that map each point \mathbf{x} in the crystal onto a point \mathbf{y} equivalent to \mathbf{x} . Clearly, in our model the lattice group

$$(9.1) \quad H = \{\mathbf{T}_a : \mathbf{a} = n_1\mathbf{b}_1 + n_2\mathbf{b}_2 + n_3\mathbf{b}_3\}$$

is a subgroup of the complete symmetry group. Now we forget about our hypothetical model and simply define an ideal crystal as a solid (filling all space) which satisfies the **lattice postulate**: There exist noncoplanar vectors $\mathbf{b}_1, \mathbf{b}_2, \mathbf{b}_3$ such that any point \mathbf{x} is equivalent to all points

$$(9.2) \quad \mathbf{x} + n_1\mathbf{b}_1 + n_2\mathbf{b}_2 + n_3\mathbf{b}_3, \quad n_1, n_2, n_3 \text{ integers.}$$

The lattice postulate amounts to the requirement that the lattice group H given by (9.1) is a symmetry group of the crystal. In addition we require that H is the maximal lattice symmetry group of the crystal, i.e., if \mathbf{T} is a translational symmetry then $\mathbf{T} \in H$.

Let G be the complete symmetry group of a crystal. Clearly, H is a subgroup of G ; in fact we shall see that it is a normal subgroup. G is called a **crystal group** or **space group**. A list of the possible isomorphism classes of space groups serves as a list of possible symmetry types of ideal crystals. Such a list is important because it serves as a classification scheme (something like the periodic table of the elements) into which all crystals can be fit. Furthermore, to a considerable extent the symmetry of a crystal serves to determine the physical properties of the crystal.

Before proceeding to an analysis of the possible space groups G it is useful to clarify the meaning of some of the statements made above. First of all we shall be dealing exclusively with **ideal** crystals, i.e., crystals which satisfy the lattice postulate. The extent to which **real** crystals satisfy the lattice postulate is a matter for the physicist or crystallographer to determine. Although there is a great deal of evidence to support such a postulate, in the final analysis the validity of this postulate depends on experimental verification (and on the physicists definition of a crystal). We do not wish to claim that the possible crystal structures are determined *a priori* by group theory.

The H -orbit of every point \mathbf{x} in a crystal is a Bravais lattice L , (9.2). However, it is not true that the crystal can be identified with L . In particular, the elements of the holohedry F of L may not be elements of the space group

G . To understand this, think of a model of a crystal formed by placing an identical pattern of atoms about each vertex in a lattice L . The translational symmetry is completely determined by the lattice. However, the total symmetry group G is also dependent on the pattern of atoms about each lattice point. [Some of the crystal symmetries may be of the form $\mathbf{g} = \{\mathbf{a}, \mathbf{O}\}$, where $\mathbf{O} \in \mathbf{O}(3)$ is not the identity and $\mathbf{a} \notin H$. Such symmetries are screw displacements or glide reflections.]

We examine the space group G of an ideal crystal in more detail. Every $\mathbf{g} \in G$ can be written uniquely in the form

$$(9.3) \quad \mathbf{g} = \{\mathbf{a}, \mathbf{O}\} = \mathbf{T}_\mathbf{a}\mathbf{O},$$

where $\mathbf{O} \in O(3)$, the orthogonal group about $\mathbf{0}$. If $\mathbf{O} = E$ then $\{\mathbf{a}, E\} = \mathbf{T}_\mathbf{a} \in H$, i.e., \mathbf{a} can be written in the form (9.1). Since $T(3)$ is a normal subgroup of $E(3)$,

$$(9.4) \quad \mathbf{gT}_\mathbf{a}\mathbf{g}^{-1} \in T(3) \cap G = H,$$

so H is normal in G . Let K be the set of all $\mathbf{O} \in O(3)$ that occur in expression (9.3) as \mathbf{g} runs over the elements of G . The relation

$$(9.5) \quad \mathbf{g}_1\mathbf{g}_2 = \{\mathbf{a}_1, \mathbf{O}_1\}\{\mathbf{a}_2, \mathbf{O}_2\} = \{\mathbf{a}_1 + \mathbf{O}_1\mathbf{a}_2, \mathbf{O}_1\mathbf{O}_2\}$$

for $\mathbf{g}_1, \mathbf{g}_2 \in G$ proves that K is a group. (However, K may not be a subgroup of G since \mathbf{a}_1 and \mathbf{a}_2 are not necessarily in the lattice group H .) Furthermore, the identity

$$(9.6) \quad \mathbf{gT}_\mathbf{b}\mathbf{g}^{-1} = \{\mathbf{Ob}, E\} = \mathbf{T}_{\mathbf{Ob}} \in H$$

valid for \mathbf{b} in H and $\mathbf{g} \in G$ given by (9.3), shows that $\mathbf{O} \in K$ maps any lattice vector \mathbf{b} in H into another lattice vector. This proves that K is one of the 32 crystallographic point groups. Thus, to each ideal crystal we can uniquely assign a crystallographic point group K .

The group K is isomorphic to the factor group G/H . Indeed, each (left or right) H -coset of G consists of all elements of the form $\{\mathbf{a}, \mathbf{O}\}$ for some fixed $\mathbf{O} \in K$. Furthermore, if $\mathbf{g}_1 = \{\mathbf{a}_1, \mathbf{O}\}$ and $\mathbf{g}_2 = \{\mathbf{a}_2, \mathbf{O}\}$ are in G then

$$(9.7) \quad \mathbf{g}_1\mathbf{g}_2^{-1} = \{\mathbf{a}_1 - \mathbf{a}_2, E\} \in H,$$

so \mathbf{g}_1 and \mathbf{g}_2 are contained in the same coset. As a unique representative in each coset we can choose the element

$$(9.8) \quad \{\mathbf{a}', \mathbf{O}\}, \quad \mathbf{a}' = \alpha_1\mathbf{b}_1 + \alpha_2\mathbf{b}_2 + \alpha_3\mathbf{b}_3,$$

where the α_i are real numbers such that $0 \leq \alpha_i < 1$. If $\alpha_1 = \alpha_2 = \alpha_3 = 0$ then $\mathbf{O} \in G \cap K$; otherwise $\mathbf{O} \notin G$. Note that the representative of the coset H is $E = \{\mathbf{0}, E\}$.

Remark. Since $K \cong G/H$ is a finite group and H is discrete it follows that G is discrete. Therefore, every space group is discrete.

In a real crystal the lengths of the basic vectors \mathbf{b}_i are of the order of the distance between neighboring atoms of the crystal since unit cells contain comparatively few atoms. These lengths are so small that they cannot be detected by macroscopic observations. To the macroscopic observer the translational symmetry group of the crystal appears to be $T(3)$. That is, the physical properties of the crystal appear to be invariant under any translation. (Recall that we are neglecting boundary effects by assuming that the crystal occupies all space.) Similarly the vectors \mathbf{a}' in (9.8) appear to the macroscopic observer to be $\mathbf{0}$, so the elements of $K \cong G/H$ appear to form the point symmetry group of the crystal. The complete symmetry group of the crystal appears to be the semidirect product of K and $T(3)$. Thus, as far as macroscopic observations are concerned, every crystal falls into exactly one of 32 possible crystal classes determined by the crystallographic point group K .

It is only when we carry out microscopic observations which can detect the existence of a primitive cell that the space group of the crystal becomes important. In particular, microscopic observations may show that K is *not* a symmetry group of the crystal.

Two crystals belonging to the same (macroscopic) crystal class may not have isomorphic space groups. In fact, it can be shown that the 32 crystal classes break up into 219 isomorphism classes of space groups. In the next section we shall indicate how these results are obtained.

The reader may be wondering why we classified point groups in conjugacy classes and then switched to the (cruder) cataloging of space groups in isomorphism classes. The reason is a practical one. Consider those space groups which are just lattice groups, i.e., $K = \{\mathbf{E}\}$. There are already a continuum number of conjugacy classes of lattice groups, so a listing of conjugacy classes of space groups is out of the question. On the other hand, all three-dimensional lattice groups form a single isomorphism class.

2.10 Space Groups

Definition. A **crystallographic space group** (**space group**) G is a discrete subgroup of $E(3)$ such that $H = G \cap T(3)$ is a three-dimensional lattice group.

According to Eq. (9.3)–(9.6) the space group G is a symmetry group of some ideal crystal. That is, the definition of space group given above is equivalent to the more intuitive definition of a symmetry group of an ideal crystal.

It is a tedious exercise to determine all isomorphism classes of space groups. Here we discuss only the basic ideas involved in such a classification.

Every space group G belongs to one of 14 lattice types and one of 32 crystal classes determined by the lattice group H and the crystallographic point group $K \cong G/H$. Recall from Table 2.2 that the lattice type severely

restricts the possible crystal classes. In particular, a crystal class K is assigned to the lattice type with *smallest* holohedry F containing K . We shall examine the significance of this assignment shortly.

Given a lattice type H and crystal class K which leaves H invariant, we look for all space groups G with lattice subgroup H such that $G/H \cong K$. Clearly one such group is the semidirect product of K and H :

$$(10.1) \quad G = \{\mathbf{h}\mathbf{k} : \mathbf{h} \in H, \mathbf{k} \in K\}$$

$$(10.2) \quad (\mathbf{h}_1\mathbf{k}_1)(\mathbf{h}_2\mathbf{k}_2) = \mathbf{h}_1(\mathbf{k}_1\mathbf{h}_2\mathbf{k}_1^{-1})(\mathbf{k}_1\mathbf{k}_2) \in G.$$

In this case the point group K is actually a subgroup of G . Space groups of the form (10.1) are called **symmorphic groups**. There are 73 isomorphism classes of symmorphic groups.

Indeed, referring to Table 2.2, we see that the triclinic crystal system has one lattice type and two crystal classes, which yields a total of two symmorphic groups. The monoclinic system has three classes and two types, which yields six symmorphic groups, etc. Proceeding in this way, we get a total of 61 symmorphic groups. To find the remaining 12 groups, we must examine our procedure more carefully.

First we consider the reasoning behind the assignment of a crystal class K to the type with the smallest holohedry containing K . Suppose F and F' are holohedries such that $F \supset F' \supseteq K$. The reader can verify that (with one exception) a lattice type belonging to the holohedry F can always be changed to a lattice type belonging to F' by an arbitrarily small deformation of the basic lattice vectors. Thus, the semidirect product of F' and K must be isomorphic to the semidirect product of F and K , and we get no new isomorphism classes of symmorphic space groups by associating K with lattice types belonging to F . The single exception occurs in the case $F = D_{6h}$, $F' = D_{3d}$, where the lattice type Γ_h cannot be changed to type $\Gamma_{r,h}$ by an arbitrarily small deformation. In this case the five crystal classes belonging to the rhombohedral system can be combined with the hexagonal lattice group to yield five new isomorphism classes of symmorphic groups.

In certain cases the group K may act as a symmetry group of a lattice H in two physically distinct ways. This can occur if the smallest holohedry F containing K also contains another subgroup K' which is isomorphic but not conjugate to K . Then the semidirect product of K and H may not be isomorphic to the semidirect product of K' and H . For example the crystal class C_{2v} in the orthorhombic system can act on the base-centered cell Γ_o^b in two distinct ways depending on whether the twofold axis of C_{2v} is parallel or perpendicular to the lattice vector \mathbf{b}_3 . Thus, there are two symmorphic space groups G of type Γ_o^b and crystal class C_{2v} . In the tetragonal system D_{2d} is the only crystal class without a fourfold axis. It is not difficult to show that D_{2d} can operate on each of the lattice types Γ_q and Γ_q^v in two distinct

ways, yielding two more symmorphic groups. Finally each of the crystal classes C_{3v} , D_3 , D_{3d} , and D_{3h} acts on the primitive hexagonal lattice Γ_h in two distinct ways. This yields four more groups, for a total of $61 + 5 + 1 + 2 + 4 = 73$ symmorphic groups.

The nonsymmorphic space groups G have the property that they contain elements of the form (9.8) with $\mathbf{a}' \neq \mathbf{0}$. In particular the crystal class K of G is *not* a subgroup of G . Let $\mathbf{O}_1, \dots, \mathbf{O}_n$ be an enumeration of the elements of K . To find all space groups G with crystal class K and lattice group H it is enough to find all sets of vectors $\mathbf{a}_1', \dots, \mathbf{a}_n'$ such that the product of any two group elements

$$(10.3) \quad \{\mathbf{a}_1', \mathbf{O}_1\}, \dots, \{\mathbf{a}_n', \mathbf{O}_n\}$$

can be written as the product of an element of H and some one of these group elements. [The \mathbf{a}_i' are subject to the restriction (9.8). If all the \mathbf{a}_i' are zero vectors then G is symmorphic. The nonsymmorphic space groups contain nontrivial screw displacements and glide reflections.] Once all such groups are determined it is necessary to sort them into isomorphism classes. It turns out that there are 146 isomorphism classes of nonsymmorphic space groups. This gives us a total of 219 space groups. (In particular there are only a finite number of space groups. For a proof see Burckhardt [1].)

To illustrate the methods used in this classification we will compute all space groups belonging to the crystal class C_4 . Such groups must necessarily belong to the tetragonal crystal system, so the possible lattice types are primitive (Γ_q) or body-centered (Γ_q^v).

First we compute the groups of type Γ_q . Recall that the basic vectors $\mathbf{b}_1, \mathbf{b}_2, \mathbf{b}_3$ of Γ_q are mutually orthogonal, $\|\mathbf{b}_1\| = \|\mathbf{b}_2\|$, and the fourfold axis l of C_4 lies along \mathbf{b}_3 . Let \mathbf{C} be a rotation through the angle $+\pi/2$ about l . According to the remarks following (10.3) we must find all possible triples of vectors $\mathbf{a}_1, \mathbf{a}_2, \mathbf{a}_3$ with

$$(10.4) \quad \mathbf{a}_i = \sum_{j=1}^3 \alpha_{ji} \mathbf{b}_j, \quad 0 \leq \alpha_{ji} < 1, \quad i = 1, 2, 3$$

such that the product of any two of

$$(10.5) \quad \{\mathbf{0}, \mathbf{E}\}, \quad \{\mathbf{a}_1, \mathbf{C}\}, \quad \{\mathbf{a}_2, \mathbf{C}^2\}, \quad \{\mathbf{a}_3, \mathbf{C}^3\}$$

is equal to the product of an element of the lattice group H and some one of the elements (10.5). (In fact, $\{\mathbf{a}_1, \mathbf{C}\}$ and H generate the entire space group G .) Once the possible space groups have been determined they must be split into isomorphism classes.

The equation to be solved for the \mathbf{a}_i reads

$$(10.6) \quad \{\mathbf{a}_i, \mathbf{C}^i\} \{\mathbf{a}_j, \mathbf{C}^j\} = \{\mathbf{h}_{ij}, \mathbf{E}\} \{\mathbf{a}_k, \mathbf{C}^{i+j}\},$$

where $\mathbf{h}_{ij} \in H$, $k = i + j \pmod{4}$, and $\mathbf{a}_0 = \mathbf{0}$. Carrying out the indicated

multiplications in (10.6), we find

$$(10.7) \quad \mathbf{a}_i + \mathbf{C}^i \mathbf{a}_j - \mathbf{a}_k \in H, \quad 0 \leq i, j \leq 3.$$

Set $\mathbf{a}_i = \mathbf{u}_i + \mathbf{v}_i$, where \mathbf{u}_i lies along l and \mathbf{v}_i is perpendicular to l . Since $\mathbf{C}\mathbf{u}_i = \mathbf{u}_i$, Eq. (10.7) split into

$$(10.8a) \quad \mathbf{u}_i + \mathbf{u}_j - \mathbf{u}_k \in H$$

$$(10.8b) \quad \mathbf{v}_i + \mathbf{C}^i \mathbf{v}_j - \mathbf{v}_k \in H.$$

In particular expression (10.8a) is an integer multiple of \mathbf{b}_3 and (10.8b) is an integral linear combination of \mathbf{b}_1 and \mathbf{b}_2 . Since $\{\mathbf{a}_1, \mathbf{C}\}^4 \in H$ we have $4\mathbf{u}_1 = n\mathbf{b}_3 \in H$. Therefore, there are four possibilities,

$$(10.9) \quad \mathbf{u}_1 = \frac{1}{4}n\mathbf{b}_3, \quad n = 0, 1, 2, 3,$$

and the rest of the \mathbf{u}_i can be determined uniquely from \mathbf{u}_1 and (10.8a). Expressions (10.8b) are not so easy to solve. However, by making use of the fact that $\mathbf{C}^2 \mathbf{v}_j = -\mathbf{v}_j$ we can check that these expressions are equivalent to

$$(10.10) \quad \mathbf{v}_2 - \mathbf{v}_1 - \mathbf{C}\mathbf{v}_1 \in H, \quad \mathbf{v}_3 - \mathbf{C}\mathbf{v}_1 \in H.$$

Expressions (10.8b) have an infinite number of solutions, since \mathbf{v}_i can be chosen arbitrarily, in which case \mathbf{v}_2 and \mathbf{v}_3 are determined by (10.4) and (10.10).

Let G be the space group corresponding to a particular choice of \mathbf{v}_1 . Note that for any $\mathbf{T}_a \in T(3)$ the group $G' = \mathbf{T}_a G \mathbf{T}_a^{-1}$ is conjugate, hence isomorphic to G . Since $\mathbf{T}_a \mathbf{h} \mathbf{T}_a^{-1} = \mathbf{h}$ for $\mathbf{h} \in H$, G and G' have the same lattice groups. Moreover,

$$(10.11) \quad \mathbf{T}_a \{\mathbf{a}_1, \mathbf{C}\} \mathbf{T}_a^{-1} = \{\mathbf{a}_1 - \mathbf{C}\mathbf{a} + \mathbf{a}, \mathbf{C}\} = \{\mathbf{a}'_1, \mathbf{C}\}.$$

Writing $\mathbf{a}'_1 = \mathbf{u}'_1 + \mathbf{v}'_1$, we find

$$(10.12) \quad \mathbf{u}'_1 = \mathbf{u}_1, \quad \mathbf{v}'_1 = \mathbf{v}_1 - \mathbf{C}\mathbf{v}_1 + \mathbf{a}.$$

An appropriate choice of \mathbf{a} yields $\mathbf{v}'_1 = \mathbf{0}$ [set $\mathbf{a} = -\frac{1}{2}(\mathbf{v}_1 + \mathbf{C}\mathbf{v}_1)$. Thus, G is conjugate to a space group with $\mathbf{v}_1 = \mathbf{0}$. Furthermore, (10.10) implies $\mathbf{v}_2 = \mathbf{v}_3 = \mathbf{0}$. We conclude that there are at most four isomorphism classes of space groups of type Γ_q and crystal class C_4 . For each of these groups C_4^j , $j = 1, \dots, 4$, we list the element $\{\mathbf{a}_1, \mathbf{C}\}$ which, together with H , generates the group:

$$(10.13) \quad C_4^1: \{\mathbf{0}, \mathbf{C}\}, \quad C_4^2: \{\frac{1}{4}\mathbf{b}_3, \mathbf{C}\}, \quad C_4^3: \{\frac{1}{2}\mathbf{b}_3, \mathbf{C}\}, \quad C_4^4: \{\frac{3}{4}\mathbf{b}_3, \mathbf{C}\}.$$

The group C_4^1 is symmorphic, while the other groups contain nontrivial screw displacements. Instead of the generator we chose for C_4^4 we could have chosen $\{\frac{1}{4}\mathbf{b}_3, \mathbf{C}^{-1}\}$. This is called a left-handed screw displacement, just as the generator $\{\frac{1}{4}\mathbf{b}_3, \mathbf{C}\}$ of C_4^2 is called a right-handed screw displacement. It is clear that C_4^2 and C_4^4 differ only the winding-sense along their respective

screw axes. In particular C_4^2 and C_4^4 are isomorphic groups. The isomorphism acts like the identity on H and takes $\{\frac{1}{4}\mathbf{b}_3, \mathbf{C}^{-1}\}$ into $\{\frac{1}{4}\mathbf{b}_3, \mathbf{C}\}$. Isomorphic pairs of space groups differing only in their winding-sense are called **enantiomorphic**. There are 11 pairs of enantiomorphic space groups. These pairs are distinguished by crystallographers because enantiomorphic crystals turn out to have physically very different properties. Thus, crystallographers recognize 230 space groups even though there are only 219 isomorphism classes (Burckhardt [1]).

We now pass to the determination of class C_4 space groups of type Γ_q^v . Recall that the basic vectors $\mathbf{b}_1, \mathbf{b}_2, \mathbf{b}_3$ for a lattice of type Γ_q^v are chosen such that \mathbf{b}_1 and \mathbf{b}_2 are perpendicular to the fourfold axis l of C_4 , $\mathbf{b}_1 \perp \mathbf{b}_2$, $\|\mathbf{b}_1\| = \|\mathbf{b}_2\|$, and $2\mathbf{b}_3 - \mathbf{b}_1 - \mathbf{b}_2$ lies along l . We consider the elements (10.4) and (10.5) now adapted to the lattice type Γ_q^v . Then $\{\mathbf{a}_1, \mathbf{C}\}^4 = \{(\mathbf{E} + \mathbf{C} + \mathbf{C}^2 + \mathbf{C}^3)\mathbf{a}_1, \mathbf{E}\} \in H$. Furthermore, $\mathbf{C}\mathbf{b}_1 = \mathbf{b}_2$, $\mathbf{C}\mathbf{b}_2 = -\mathbf{b}_1$, $\mathbf{C}\mathbf{b}_3 = \mathbf{b}_3 - \mathbf{b}_1$. Thus, if $\mathbf{a}_1 = \alpha_1\mathbf{b}_1 + \alpha_2\mathbf{b}_2 + \alpha_3\mathbf{b}_3$ we find

$$(\mathbf{E} + \mathbf{C} + \mathbf{C}^2 + \mathbf{C}^3)\mathbf{a}_1 = 2\alpha_3(2\mathbf{b}_3 - \mathbf{b}_1 - \mathbf{b}_2) \in H.$$

The only possibilities are $\alpha_3 = 0$ or $\alpha_3 = \frac{1}{2}$. We can map G onto a conjugate space group $G' = \mathbf{T}_a G \mathbf{T}_a^{-1}$ such that the image $\{\mathbf{a}'_1, \mathbf{C}\}$ of $\{\mathbf{a}_1, \mathbf{C}\}$ is given by

$$(10.14) \quad \mathbf{a}'_1 = \mathbf{a}_1 - \mathbf{C}\mathbf{a} + \mathbf{a} = \alpha'_1\mathbf{b}_1 + \alpha'_2\mathbf{b}_2 + \alpha'_3\mathbf{b}_3.$$

By choosing $\mathbf{a} \in R_3$ appropriately we can require that α'_1 and α'_2 take any desired values. [Note that $(\mathbf{a} - \mathbf{C}\mathbf{a}) \perp l$.] In the case $\alpha_3 = 0$ we choose $\alpha'_1 = \alpha'_2 = 0$ and obtain the symmorphic group

$$(10.15) \quad C_4^5: \quad \{\mathbf{0}, \mathbf{C}\}.$$

In the case $\alpha_3 = \frac{1}{2}$ it is most convenient to choose $\alpha'_1 = \alpha'_2 = -\frac{1}{4}$ so $\mathbf{a}'_1 = \frac{1}{4}\mathbf{b}_4$, where $\mathbf{b}_4 = 2\mathbf{b}_3 - \mathbf{b}_1 - \mathbf{b}_2$. It is trivial to verify that $\{\frac{1}{4}\mathbf{b}_4, \mathbf{C}\}$ and H generate the space group

$$(10.16) \quad C_4^6: \quad \{\frac{1}{4}\mathbf{b}_4, \mathbf{C}\}.$$

We have shown that there are six space groups of crystal class C_4 (five isomorphism classes). The techniques used to derive these results are typical of those used to obtain the complete list of space groups.

Problems

- 2.1 Using only the definition (2.1), show that an isometry \mathbf{T} maps a line segment with endpoints $\mathbf{x}_1, \mathbf{x}_2$ onto a line segment with endpoints $\mathbf{T}\mathbf{x}_1, \mathbf{T}\mathbf{x}_2$. Then show that \mathbf{T} maps planes onto planes.
- 2.2 Prove: An isometry which fixes four noncoplanar points is the identity transformation.
- 2.3 Compute all point groups in two-dimensional space. (Answer: $C_n, D_n, n = 1, 2, \dots$)

- 2.4 Show that there are exactly two space groups belonging to crystal class C_{6h} .
2.5 Show that there are exactly four space groups belonging to crystal class D_{3h} .

The next three problems concern two-dimensional lattices and space groups. They are much simpler than the corresponding problems in three-space.

- 2.6 Prove that there are ten crystallographic point groups in the plane.
2.7 Verify that there are four holohedries C_2 , D_2 , D_4 , and D_6 and six two-dimensional lattice types.
2.8 Verify the existence of exactly 13 isomorphism classes of symmorphic two-dimensional space groups and 4 nonsymmorphic groups.
2.9 Let $O'(3) = O(3) \times [E, R]$, where $R^2 = E$ and E is the identity operator. A **magnetic symmetry group (color group)** is a finite subgroup G of $O'(3)$ such that $O \in O(3)$ satisfies the crystallographic restriction for each $g = O \times E$ or $g = O \times R$ in G . Using the proof of Theorem 2.5, show that the magnetic symmetry groups G fall into three classes: (1) the 32 crystallographic point groups, i.e., $G \subset O(3)$; (2) the 32 groups $K \times [E, R]$, where K is a crystallographic point group, i.e., $R \in G$; (3) groups G such that $R \notin G$ but $G \not\subset O(3)$. Show how to determine (in principle) all 58 groups in class (3). What is the physical significance of these groups? (See Hamermesh [1].)
2.10 Explain the rationale behind the Schöenflies notation for point groups, especially the meaning of the subscripts d , h , and n .
2.11 Prove Corollaries 2.3 and 2.4.