Point Groups and Crystal Systems

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Symmetry is a powerful tool in solid-state physics. All crystals can be classified by symmetry. The following is a summary of the theory of symmetry in crystals. A complete discussion of finite point groups and crystal systems is presented, plus a brief overview of space groups and the representations of the symmetry groups.

1 Point Groups

A *point group* is a group of symmetries that leaves at least one point in space fixed, that is, a subgroup of the orthogonal group $O(N)$, where N is the dimension of the space. The elements of a point group are usually called *point symmetries*. Point symmetries are useful in chemistry in describing molecules. Although molecules are not our interests here, the following sections are devoted to thorough discussion of the theory of point groups because it is indispensable for the classification of crystal lattices. We shall only consider *finite* point groups since a lattice cannot possess infinite point symmetries.

1.1 Point Symmetry Operations

We will use the Schoenflies notation to indicate the symmetry elements. Every point symmetry operation belongs to one of the following categories:

E. Identity.

C_n. Rotation by an angle $2\pi/n$ about an axis (called an *n-fold axis* and usually denoted by just n). In 2 dimensions the axis should be taken perpendicular to the plane. Note that C_1 is the same as identity ($C_1 = E$).

σ. Reflection about a plane (called the *mirror* and denoted by m). In 2 dimensions the mirror should be taken perpendicular to the plane.

i. Inversion with respect to a point (called the *inversion center*). Note that in 2 dimensions inversion is the same as rotation by π ($i = C_2$), and that in 3 dimensions an inversion is the same as a rotation by π followed by a reflection about a plane perpendicular to the axis ($i = S_2$, see below).

S_n. *Improper rotation*, defined to be a rotation C_n (sometimes called a *proper* rotation) followed by a reflection about a plane perpendiculat to the axis (so S_n is only defined in 3 dimensions). See Figure 1. It is easy to see that the two operations commute, so $S_n = C_n \cdot \sigma = \sigma \cdot C_n$. As noted above, S_2 is the

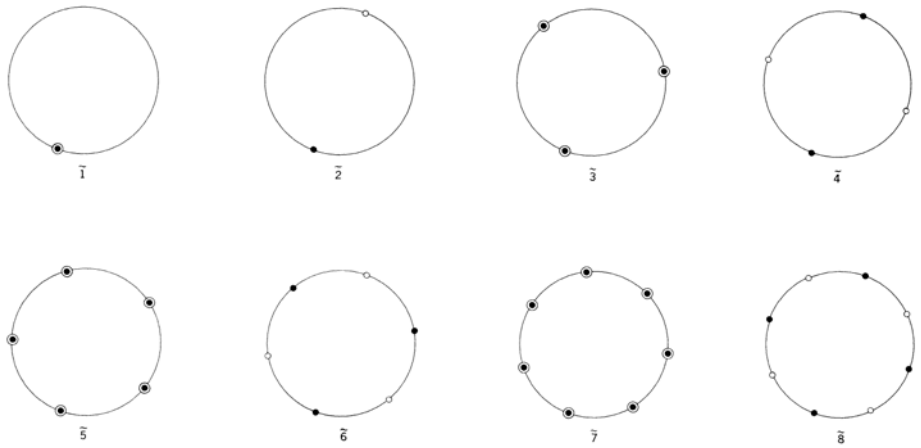


Figure 1 Improper Rotations. •'s represent points above the plane and ∘'s represent points below the plane.

same as inversion ($S_2 = i$). Also, since C_1 is identity, S_1 is the same as pure reflection ($S_1 = \sigma$).

1.2 Conbinations of Point Symmetry Operations

We show some important results of two successive operations. Here we focus on 3 dimensions. The 2-D case is a simplification of the following discussion.

Combination of two rotations. Since point symmetries must leave one point in space fixed, we only consider rotations with intersecting axes. The combination of such rotations is another rotation. This can be easily seen by looking at the motion of points on the unit sphere centered at the intersection O of the axes (Figure 2). In the figure, a rotation by α about OA followed by a rotation by β about OB yields a rotation by γ about OC. If we define the positive directions of α, β, γ properly, then in a shorthand way, we can write $B_\beta \cdot A_\alpha = C_{-\gamma}$, or

$$C_\gamma \cdot B_\beta \cdot A_\alpha = E.$$

This relation should be read in the sense that whenever two of the operations are given, the third follows.

By elementary spherical trigonometry, it can be proved that the angles satisfy the following formula:

$$\cos w = \frac{\cos\frac{\gamma}{2} + \cos\frac{\alpha}{2}\cos\frac{\beta}{2}}{\sin\frac{\alpha}{2}\sin\frac{\beta}{2}} \tag{1}$$

where w is the angle between OA and OB. Since $\cos w$ should be between -1 and 1, the angles α, β, γ cannot take arbitrary values. Furthermore, for finite

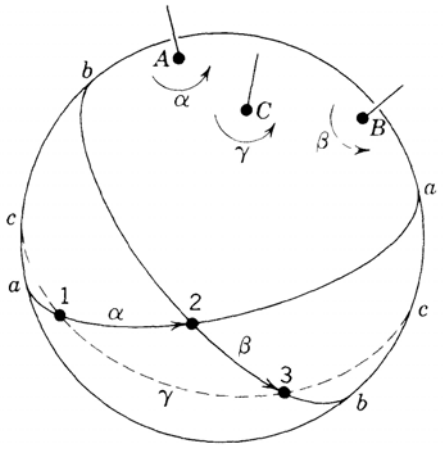


Figure 2 Combination of two rotations.

point groups α, β, γ must all be 2π divided by some integers, so there is an even stronger restriction on the rotational symmetries a system can simultaneous have. For example, a system cannot have a 4-fold axis and a 3-fold axis in perpendicular, for if we take $\alpha = \pi/2, \beta = 2\pi/3$, and $w = \pi/2$ in (1), we get $\gamma = \cos^{-1}(-3/4)$, which is not commensurable with 2π and thus will generate an infinite group.

Combination of two reflections. A reflection about the mirror m_1 followed by a reflection about the mirror m_2 yields a rotation by 2μ about the line of intersection A of m_1 and m_2, where μ is the angle between the two mirrors (Figure 3). In a shorthand way, we write $\sigma_2 \cdot \sigma_1 = A_{2\mu}$, or

$$A_{-2\mu} \cdot \sigma_2 \cdot \sigma_1 = E.$$

Again, this relation should be read in the sense that whenever two of the operations are given, the third follows. Thus the combination of a rotation and a reflection about a mirror containing the axis of rotation is a reflection about another mirror containing the axis such that the angle between the mirrors is half the angle of rotation.

Combination of a rotation and an inversion. Due to the requirement that a point in space is fixed, the axis of rotation must pass through the inversion center. The result is an improper rotation (Figure 4). By comparing Figure 4 and Figure 1, we have the relations $i \cdot C_n = S_{2n}^{-1}$ if n is odd, $i \cdot C_n = S_{\frac{n}{2}}^{-1}$ if $n = 4k + 2$ for some $k \in \mathbb{N}$, and $i \cdot C_n = S_n$ if $n = 4k$ for some $k \in \mathbb{N}$, or

$$S_{2n} \cdot i \cdot C_n = E \quad \text{if } n \text{ is odd}$$

$$S_{\frac{n}{2}} \cdot i \cdot C_n = E \quad \text{if } n = 4k + 2 \text{ for some } k \in \mathbb{N}$$

$$S_n \cdot i \cdot C_n = E \quad \text{if } n = 4k \text{ for some } k \in \mathbb{N}$$

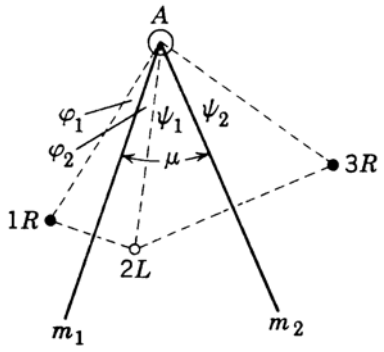


Figure 3 Combination of two reflections.

As before, these relations should be read in the sense that whenever two of the symmetry elements are given, the third follows. Note that by taking $n = 1$, we see that the combination of an inversion and a reflection (S_1) such that the mirror contains the inversion center is a rotation by π (C_2) about the line passing through the inversion center and perpendicular to the mirror.

1.3 Classification of Finite 2-D and 3-D Point Groups

The relations derived in 1.2 reduce the work of classifying finite point groups significantly. The complete classification is recorded here.

All finite 2-D point groups belong to one of the two infinite series C_n and

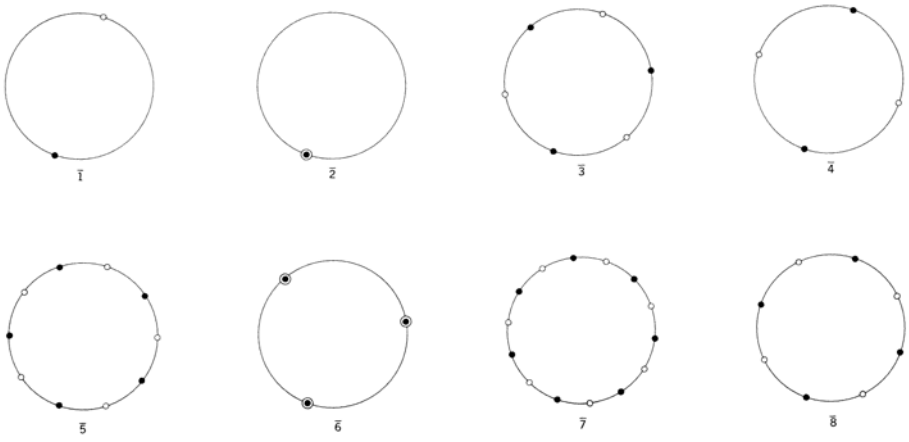


Figure 4 Combination of a rotation and an inversion.

D_n. The *cyclic group* C_n consists of elements $E, C_n, C_n^2, ..., C_n^{n-1}$ (note that C_n denotes both the group and the symmetry operation.) The *dihedral group* D_n is generated by the rotation C_n and a reflection σ. Note that given a mirror containing an n-fold axis, there must be $n-1$ other mirrors, each one separated from the neighboring mirrors by an angle π/n. Hence in D_n there are totally n reflections. The D_n thus contains $2n$ elements.

In three dimensions, up to conjugacy all of the finite point groups belong to one of the eight infinite series $C_n, C_{nh}, C_{ni}, C_{nv}, S_n, D_n, D_{nh}, D_{nd}$ except for seven high symmetry groups $T, T_d, T_h, O, O_h, I, I_h$. These families are characterized as follows. (Note that the meaning of D_n is different from that in the 2-D case.)

C_n is the cyclic group of order n, consisting of $E, C_n, C_n^2, \ldots, C_n^{n-1}$.

C_{nh} is obtained by adding to C_n a mirror perpendicular to the n-fold axis. It has $2n$ elements. Note that when n is even, the group automatically contains an inversion center (because the combination of a reflection and a rotation by π about the axis perpendicular to the mirror is an inversion.) When $n = 1$, it is usually denoted by C_s rather than C_{1h}.

C_{ni} is obtained by adding to C_n an inversion center (which must lie on the axis of rotation). As we see above, C_{nh} already contains an inversion center when n is even, so in this case C_{ni} and C_{nh} are the same. When n is odd, they are different. The C_{ni} group has $2n$ elements. When $n = 1$, it is usually denoted by C_i.

C_{nv} is obtained by adding to C_n n mirrors containing the n-fold axis. It has $2n$ elements. When $n = 1$, it is easy to see that $C_{1v} = C_{1h} = C_s$.

S_n is the group generated by the improper rotation S_n. Note that the group S_n does not necessarily contain C_n as a subgroup. The group S_n is the same as C_{nh} when n is odd and the same as $C_{\frac{n}{2}i}$ when $n = 4k + 2$ for some $k \in \mathbb{N}$ (cf. Figure 1). When n divides 4, however, S_n is different form any of the above groups. The group S_n has $[2, n]$ (the least common multiple of 2 and n) elements.

D_n is obtained by adding to C_n n 2-fold axes perpendicular to the n-fold axis. It has $2n$ elements.

D_{nh} is obtained by adding to D_n a mirror perpendicular to the n-fold axis. It has $4n$ elements. Note that the combination of the n 2-fold axes and the mirror containing them gives n mirrors, each containing the n-fold axis and one of the 2-fold axes, so equivalently we can say D_{nh} is obtained by adding to D_n these n mirrors. Like C_{nh}, D_{nh} contains an inversion center if n is even.

D_{nd} is obtained by adding to D_n n mirrors, each containing the n-fold axis and lying *between* two 2-fold axes. It has $4n$ elements. When n is odd, there will be a mirror perpendicular to each 2-fold axis, and their combination yields an inversion. Hence D_{nd} contains an inversion center if n is odd.

T is the group of the rotatinal symmetries of a regular tetrahedron. It contains four 3-fold axes (each through a vertex) and three 2-fold axes (each bisecting a pair of opposite edges). The group T has 12 elements.

T_d is obtained by adding to T six mirrors, each containing an edge and bisecting the opposite edge. It is the full tetrahedral symmetry group and has

24 elements.

T_h is obtained by adding to T an inversion center. It has 24 elements.

O is the group of the rotatinal symmetries of a regular octahedron or a cube. It contains three 4-fold axes, four 3-fold axes, and six 2-fold axes. The group O has 24 elements.

O_h is obtained by adding to O an inversion center. It is the full octahedral or cubic symmetry group and has 48 elements.

I is the group of the rotatinal symmetries of a regular icosahedron or a regular dodecahedron. It contains six 5-fold axes, ten 3-fold axes, and fifteen 2-fold axes. The group I has 60 elements.

I_h is obtained by adding to I an inversion center. It is the full icosahedral or dodecahedral symmetry group and has 120 elements.

2 Crystal Systems

2.1 Translational Symmetry

A crystal consists of atoms that repeat a translationally periodical pattern in space. (We think of crystals ideally, of course. Any real crystal has a finite size.) We say two points in the crystal are equivalent if their environment are the same, i.e. if they are indistinguishable by their surroundings. Fix a point in space. Then all points equivalent to this reference point form a *lattice*. Each of these points is called a *lattice point*. If we connect the lattice points with straight lines we will divide the space into infinitely many *unit cells*. The corners of the unit cell are the lattice points. In 3 dimensions, the unit cell is a parallelepiped, and thus can be specified by the length a, b, c of its edges and the angle α, β, γ between the edges (Figure 5). The distances a, b, c are the units of translational symmetry; that is, the system is invariant under translations of a, b, c along the corresponding directions, or their combinations. A position inside the unit cell

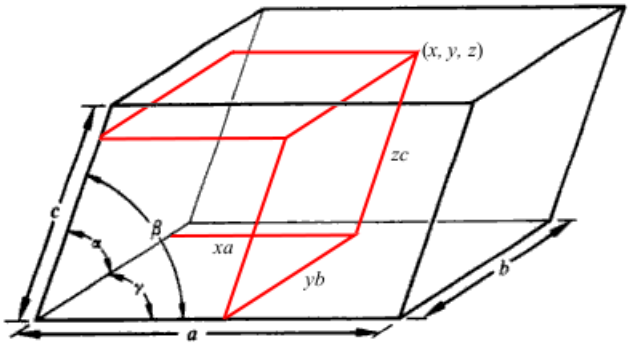


Figure 5 The unit cell.

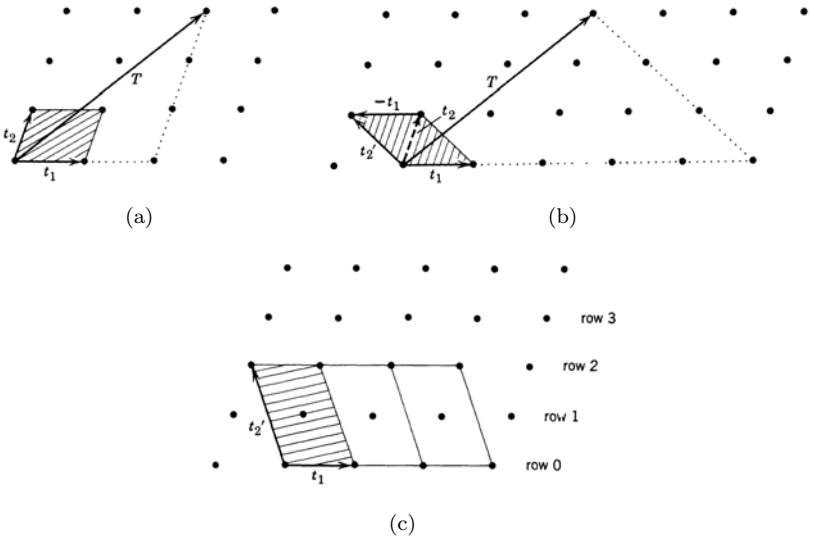


Figure 6 (a)(b) Different ways to choose the unit cell.
(c) A "double" unit cell.

can be described by a 3-tuple (x, y, z) where $0 \leq x, y, z < 1$, meaning that we can get to that position by starting from the lattice point and moving the distances xa, yb, zc parallel to the first, the second, and the third edges, respectively. Note that given a lattice there are infinite many ways to choose the unit cell (Figure 6(a)(b)). It is even permissible to have lattice points inside the unit cell (Figure 6(c)). The unit cell is called *primitive* if it has no lattice point inside; otherwise it is *centered*.

It should be expected that not all point symmetries can be satisfied by a lattice since only a few of them are compatible with translational symmetry. Consider the 2-D case. Suppose the 2-D lattice satisfies some rotational symmetry C_n. For convenience we choose our reference point to be the n-fold axis. By translational symmetry the lattice points equivalent to this point are also n-fold axes. In Figure 7 all points are n-fold axes. The two points B', C' are obtained from B, C through a single rotation by an angle $2\pi/n$ about A, D, respectively. The lattice structure requires $AD = la$ and $B'C' = ma$ for some $l, m \in \mathbb{N}$, where a is the distance between A and B. From the geometry of the figure we have

$$B'C' = AD - 2a\cos\frac{2\pi}{n}.$$

Hence

$$\cos\frac{2\pi}{n} = \frac{l-m}{2}.$$

But $\cos\frac{2\pi}{n}$ should be between -1 and 1, so the only valid values of $l - m$ are $2, 1, 0, -1, -2$, in which cases we get $n = 1, 6, 4, 3, 2$, respectively. Therefore

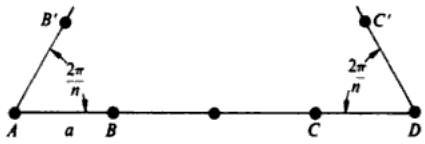


Figure 7

the only rotational symmetries a lattice can satisfy are C_1, C_2, C_3, C_4, C_6. The corresponding dihedral symmetries D_1, D_2, D_3, D_4, D_6 are also permissible since we can picture lattices satisfying these symmetries easily. These are the only 10 point groups that may be consistent with the 2-D lattice.

2.2 The 32 Crystal Classes

Now let's turn to the 3-D case. Suppose the lattice has a rotational symmetry C_n. Fix a point on the axis of rotation. It is easy to see that the plane perpendicular to the axis and containing this point also contains infinitely many lattice point equivalent to it. These points thus form a 2-D lattice. The 2-D lattice in the plane has to be invariant under rotation about the axis. It is immediate then that in the 3-D case the possible values of n are also $1, 2, 3, 4, 6$. The only difference is that a 3-D lattice may possess multiple rotational symmetries. Recall the cimbination of two rotational axis always yields the third and their relation is restricted by Equation (1). We can use a set of three numbers to denote different ways of combinations. For example, 234 means a 2-fold axis and a 3-fold axis that yield a 4-ford axis. There are only six permissible combinations: 222, 223, 224, 226, 233, 234 (Figure 8). The angles between the axes are given by (1). The first four combinations generate the dihedral groups. The combination 233 gives the tetrahedral group, and 234 gives the octahedral group (Figure 9). The five cyclic groups C_1, C_2, C_3, C_4, C_6 and the six combinations D_2, D_3, D_4, D_6, T, O are the only point groups a lattice can satisfy that contain only rotations. The first two rows of Figure 10 are these groups. The third row has only one group S_4, which is generated by the improper rotation S_4. The remaining groups can be found by adding mirrors or inversion centers to the first 12 groups. These are the only possible point symmetries of a 3-D lattice. There are 32 of them. They are called the *crystallographic point groups* or often referred to as the "32 crystal classes" in crystallography.

2.3 Lattice Types—The 2-D Case

So far we have only discussed the possible symmetries of a lattice. It is useful to know which shape of the unit cell are required for compatibility with certain symmetry. Different shapes of lattices are called the *lattice types*. In this section we shall focus on the 2-D case. The 3-D case will be dealt with in the next section. Although it might seem unnecessary here, let's first study the

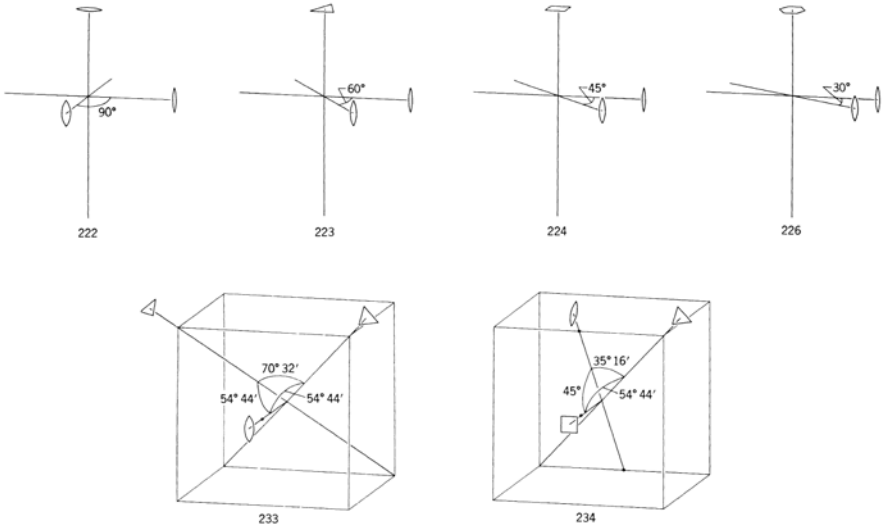


Figure 8 The six permissible crystallographic combinations of rotations.

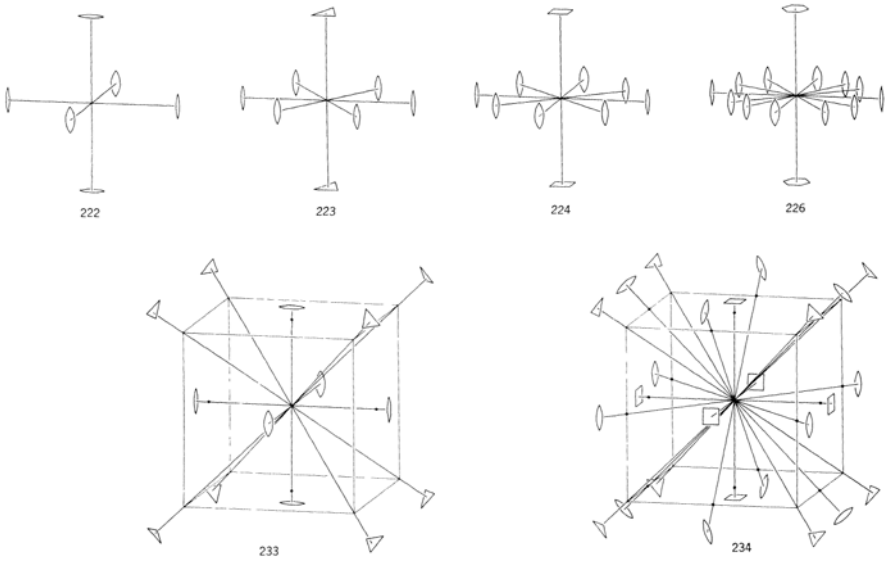


Figure 9 The six rotational symmetry groups based on Figure 8.

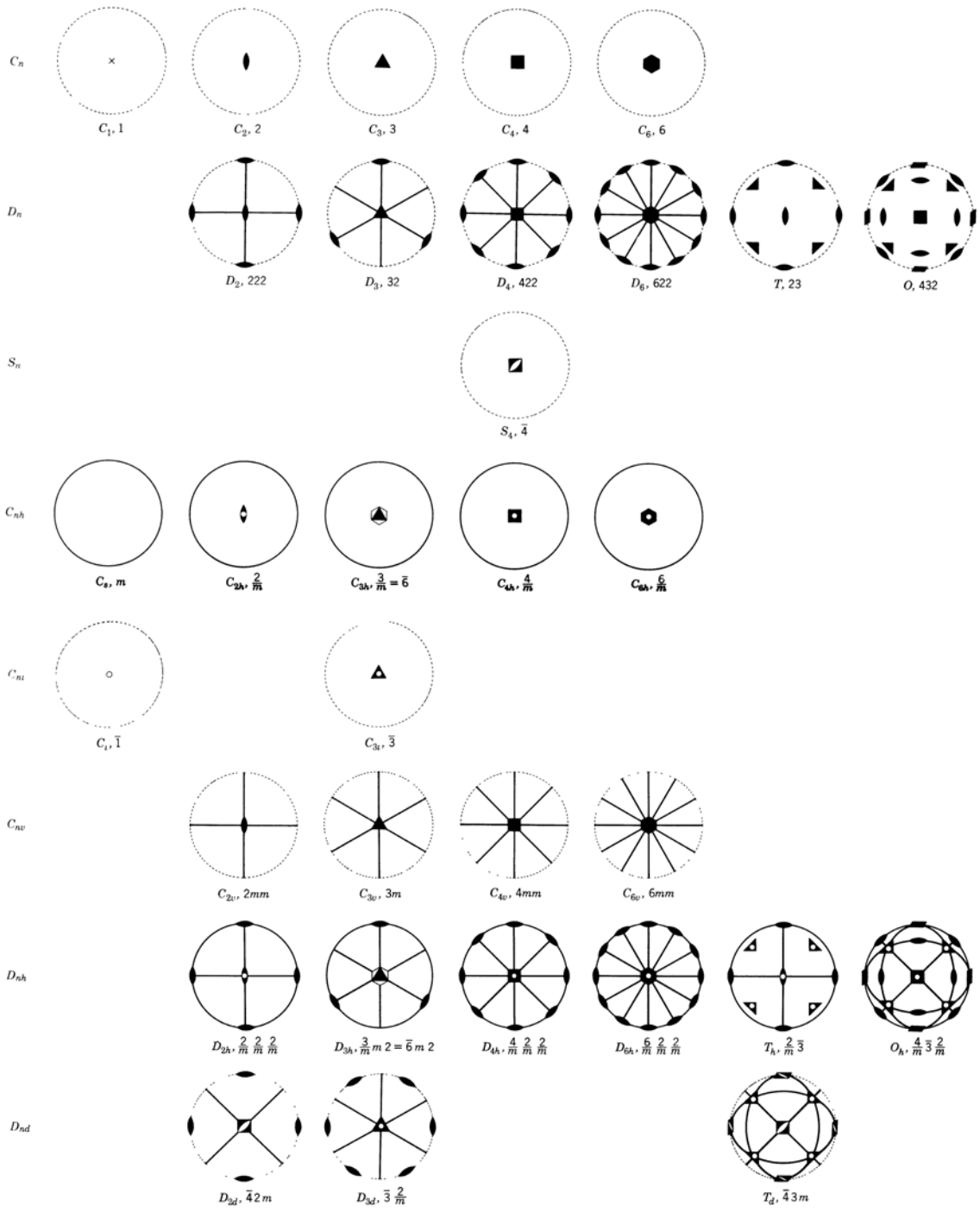


Figure 10 The 32 crystal classes.

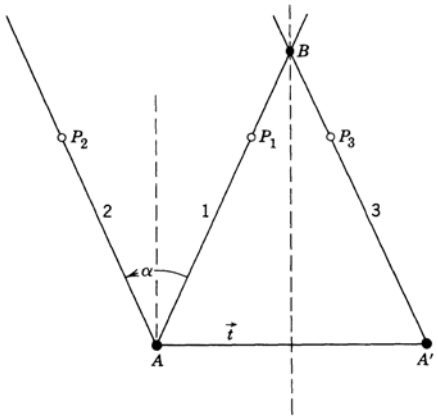


Figure 11 Combination of a rotation and a translation perpendicular to the axis of rotation.

combination of a rotation of the plane and a translation. It will be crucial in the later discussion of the 3-D case.

Figure 11 shows that a rotation by α about the axis A followed by a translation which brings A to A' yields a rotation by the same angle about the axis B on the perpendicular bisector of the segment AA'. This result can be applied directly to the lattice that has rotational symmetry. Choose the lattice points to be the equivalent rotational axes on the plane, the above result assures that there must be some *nonequivalent* axes inside the unit cell, as shown in the first five diagrams of Figure 12. They also show the required shape of the unit cell to be consistent with each symmetry. For C_1 and C_2 it can be any parallelogram, for C_3 and C_6 it has to be a 120°-rhombus, and for C_4 it need to be a square.

Next let's consider the lattice that possesses reflectional symmetry. Note that the shape of the lattice which satisfies C_3, C_4, or C_6 already has D_3, D_4, D_6 symmetries, respectively. For D_2 and D_1, they are inherently the same, since as far as the shape is concerned, a lattice consistent with reflectional symmetry must have a 2-fold axis. It can be easily seen that the only shapes that satisfy D_2 symmetry are the rectangle (where the mirrors bisect the sides of the unit cell) and the rhombus (where the mirrors contain the lattice points) as shown in the last two diagrams of Figure 12. There are thus five 2-D lattice types in total.

2.4 Lattice Types—The 3-D Case

For convenience let's fix a point on the principal axis (the axis of rotation of the highest order) and look at the lattice points equivalent to it. The 3-D lattice can be thought of as a stack of infinite many layers of 2-D lattices. We choose the layers to be perpendicular to the principal axis. Pick one of the layers and

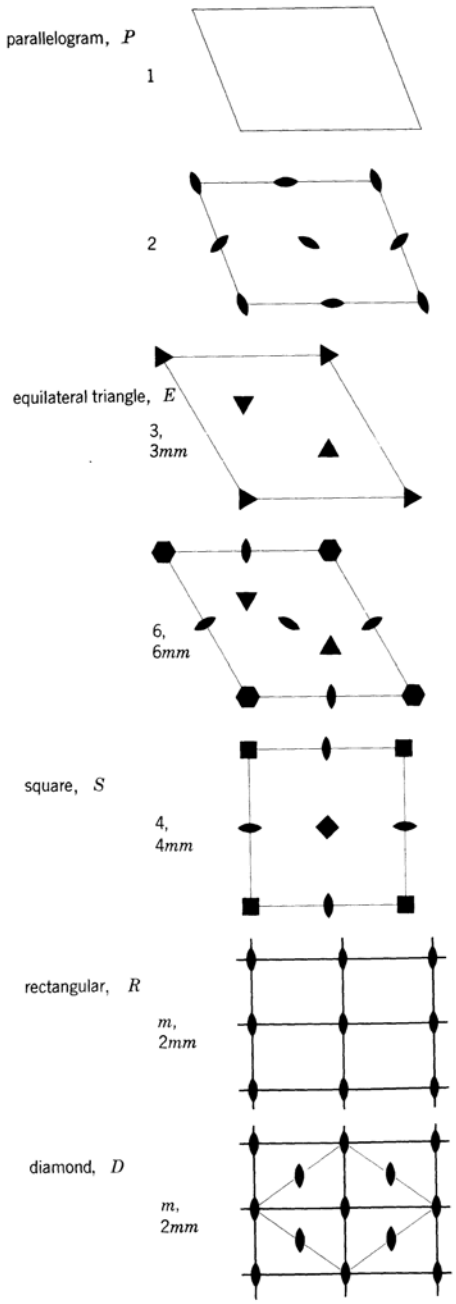


Figure 12 The distribution of axes of rotation and mirrors in the five 2-D lattice types.

call it the "ground layer" and one of its neighbering layers the "first layer." We can now describe the lattice by the position of the lattice point of the first layer relative to the unit cell of the ground layer. There are only finitely many possibilities because an n-fold axis of the ground layer must also be an n-fold axis of the first layer. The shape of the 2-D lattice of each layer is one of those given in the last section. We shall deal with them one by one.

1. The layers satisfy C_1 (any parallelogram). There is no restriction. The lattice point of the first layer can be at any position (x, y, z) relative to the unit cell of ground layer. This gives the *triclinic lattice*.

2. The layers satisfy C_2 (any parallelogram). The lattice point of the first layer can be at positions $(0, 0, z)$, $(\frac{1}{2}, \frac{1}{2}, z)$, $(0, \frac{1}{2}, z)$, or $(\frac{1}{2}, 0, z)$ relative to the unit cell of the ground layer, because these positions are above the nonequivalent 2-fold axes inside the unit cell of the ground layer (cf. Figure 12) and there is no restriction on the seperation between the two layers. The first possibility yields the *primitive monoclinic lattice* and the other three yield the *base-centered monoclinic lattice*. The choice of the unit cell for the base-centered lattice is not primitive. However, it has the advantage that two of the angles α, β, γ are $\pi/2$. It is *by virtue of symmetry* that there is always a way for a lattice satisfying C_2 to choose the unit cell so that two of the three angles are $\pi/2$.

3. The layers satisfy D_2 (rectangle or rhombus). If the 2-D lattice is rectangular, the lattice point of the first layer can be at positions $(0, 0, z)$, $(\frac{1}{2}, \frac{1}{2}, z)$, $(0, \frac{1}{2}, z)$, or $(\frac{1}{2}, 0, z)$ relative to the unit cell of the ground layer. The first possibility yields the *primitive orthorhombic lattice*, the second yields the *body-centered orthorhombic lattice*, and the other two yield the *base-centered orthorhombic lattice*. If the 2-D lattice is diamond, the lattice point of the first layer can be at positions $(0, 0, z)$ or $(\frac{1}{2}, \frac{1}{2}, z)$ relative to the unit cell of the ground layer. The first possibility still gives the base-centered orthorhombic lattice, and the second gives the *face-centered orthorhombic lattice*.

4. The layers satisfy C_4 (square). the lattice point of the first layer can be at positions $(0, 0, z)$ or $(\frac{1}{2}, \frac{1}{2}, z)$ relative to the unit cell of the ground layer. The first possibility yields the *primitive tetragonal lattice*, and the second yields the *body-centered tetragonal lattice*.

5. The layers satisfy C_3 (120°-rhombus). The lattice point of the first layer can be at positions $(0, 0, z)$, $(\frac{1}{3}, \frac{2}{3}, z)$, or $(\frac{2}{3}, \frac{1}{2}, z)$ relative to the unit cell of the ground layer. The first possibility yields the *hexagonal lattice* and the other two yield the *rhombohedral lattice*.

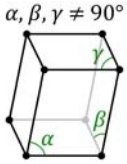
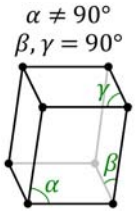
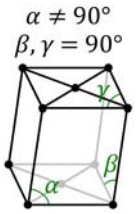
The C_6 case coincides with the first possibility of the C_3 case and so is omitted here. The only cases we miss in the above discussion are lattices with high symmetry (T and O). The extra symmetry puts restriction on the separation between the two layers. Depending on the orientation of the layers and the

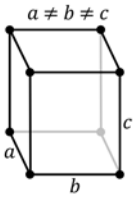
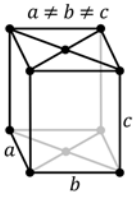
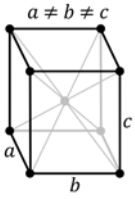
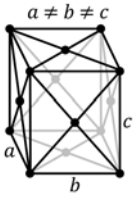
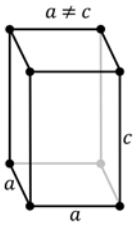
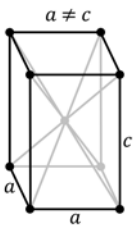
position of the lattice point of the first layer relative to the unit cell of the ground layer, the two symmetry groups give three possible lattices: the *primitive*, the *body-centered*, and the *face-centered cubic lattices*.

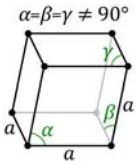
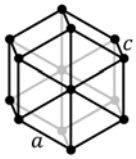
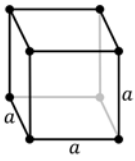
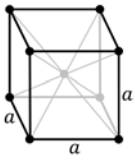
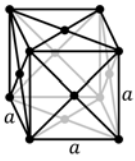
All of the above gives a total number of 14 possible 3-D lattice types. These are the so-called 14 *Bravais lattices* in crystallography.

2.5 The 7 Crystal Systems

The 14 lattice types discussed in the last section fall into 7 *crystal systems*: triclinic, monoclinic, orthorhombic, tetragonal, rhombohedral (also called *trigonal*), hexagonal, and cubic. It is now an easy task to verify which point groups each crystal system satisfies. The results are summarized in the following table. The table thus contains the complete classification of 3-D lattices.

Crystal system	**Crystal classes**	**Lattice types**
Triclinic	C_1, C_i	
Monoclinic	C_{1h}, C_2, C_{2h}	 (primitive)  (base-centered)

Orthorhombic	C_{2v}, D_2, D_{2h}	 (primitive)  (base-centered)  (body-centered)  (face-centered)
Tetragonal	$C_4, C_{4h}, C_{4v}, S_4,$ D_{2d}, D_4, D_{4h}	 (primitive)  (body-centered)

Trigonal	C_3, C_{3i}, C_{3v}, D_3, D_{3d}		
Hexagonal	$C_{3h}, C_6, C_{6h}, C_{6v}$, D_{3h}, D_6, D_{6h}		
Cubic	T, T_d, T_h, O, O_h		(primitive)
			(body-centered)
			(face-centered)
Total:			
7	32		14

3 Space Groups

The story about lattices is complete. However, there are more symmetries to describe a crystal, for the pattern can repeat *inside* the unit cell. This can be achieved by two types of symmetry operations which we haven't discussed up to this point: screws and glides.

A *screw* is the combination of a rotation and a translation *along* the axis of rotation (called the *screw axis*). The notation of the screw axis is n_p, meaning that each operation is the combination of a rotation by an angle $2\pi/n$ and a translation of p/n times the distance of translational symmetry along the axis (Figure 13). It is obvious that there is no screw operation in the 2-D case.

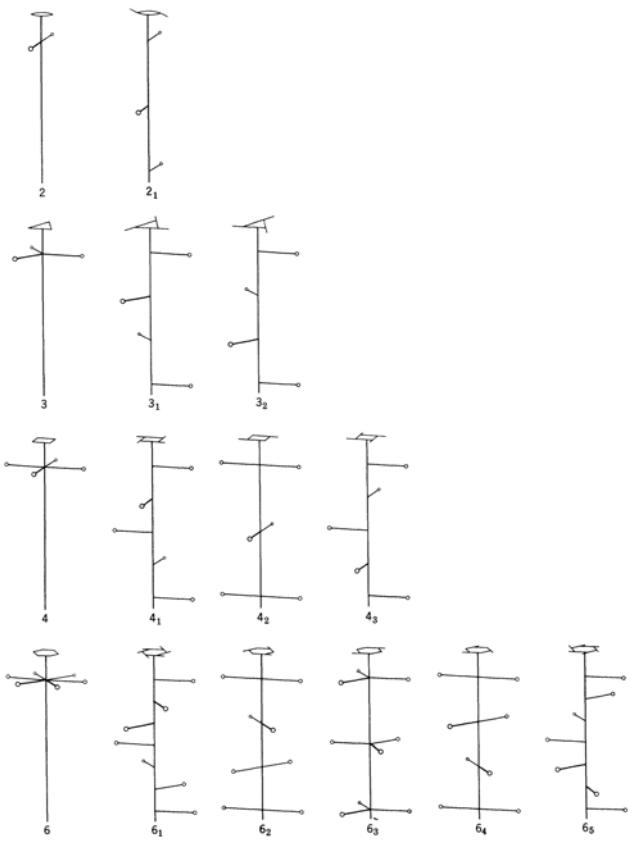


Figure 13 Illustration of screws.

A *glide* is the combination of a reflection and a translation parallel with the mirror (called the *glide plane*). Depending on the orientation of the glide plane, the glide can be *axial* or *diagonal*. For certain lattice types there can be more orientations.

Groups consisting of point symmetries, translational symmetries of the unit cell, screws, glides, and their combinations are called the *wallpaper groups* in the 2-D case and the *space groups* in the 3-D case. There are totally 17 wallpaper groups and 230 space groups. They can be studied and classified through lattice types and point groups. Detailed discussion of the wallpaper groups and the space groups can be found in Armstrong [1] and Buerger [3], respectively.

4 Representations of Point Groups and Space Groups

In practical applications the above information about the symmetry of the crystal is not enough. In order to determine the physical properties of the crystal we need to know the character tables of the symmetry groups. In Bradley and Cracknell [2] all character tables of crystallographic point groups and space groups are given, including all of the single-valued and double-valued representations.

References

[1] Armstrong, M. A. *Groups and Symmetry*. New York: Springer, 1988.

[2] Bradley, C. J. and A. P. Cracknell. *The Mathematical Theory of Symmetry in Solids: Representation Theory for Point Groups and Space Groups*. Oxford: Clarendon Press, 1972.

[3] Buerger, M. J. *Elementary Crystallography: An Introduction to the Fundamental Geometrical Features of Crystals*. New York: John Wiley & Sons, 1956.

[4] Sands, Donald E. *Introduction to Crystallography*. Mineola: Dover, 1993.

[5] Tinkham, Michael. *Group Theory and Quantum Mechanics*. Mineola: Dover, 2003.