7
Classification of Bravais Lattices and Crystal Structures

Symmetry Operations and the Classification of Bravais Lattices

The Seven Crystal Systems and Fourteen Bravais Lattices

Crystallographic Point Groups and Space Groups

Schoenflies and International Notations

Examples from the Elements

In Chapters 4 and 5, only the *translational* symmetries of Bravais lattices were described and exploited. For example, the existence and basic properties of the reciprocal lattice depend only on the existence of three primitive direct lattice vectors $\mathbf{a}_i$, and not on any special relations that may hold among them.[1] The translational symmetries are by far the most important for the general theory of solids. It is nevertheless clear from examples already described that Bravais lattices do fall naturally into categories on the basis of symmetries other than translational. Simple hexagonal Bravais lattices, for example, regardless of the c/a ratio, bear a closer resemblance to one another than they do to any of the three types of cubic Bravais lattice we have described.

It is the subject of crystallography to make such distinctions systematic and precise.[2] Here we shall only indicate the basis for the rather elaborate crystallographic classifications, giving some of the major categories and the language by which they are described. In most applications what matters are the features of particular cases, rather than a systematic general theory, so few solid state physicists need master the full analysis of crystallography. Indeed, the reader with little taste for the subject can skip this chapter entirely with little loss in understanding what follows, referring back to it on occasion for the elucidation of arcane terms.

THE CLASSIFICATION OF BRAVAIS LATTICES

The problem of classifying all possible crystal structures is too complex to approach directly, and we first consider only the classification of Bravais lattices.[3] From the point of view of symmetry, a Bravais lattice is characterized by the specification of all rigid operations[4] that take the lattice into itself. This set of operations is known as the *symmetry group* or *space group* of the Bravais lattice.[5]

The operations in the symmetry group of a Bravais lattice include all translations through lattice vectors. In addition, however, there will in general be rotations, reflections, and inversions[6] that take the lattice into itself. A cubic Bravais lattice, for example, is taken into itself by a rotation through 90° about a line of lattice points in a $\langle 100\rangle$ direction, a rotation through 120° about a line of lattice points in a $\langle 111\rangle$ direction, reflection of all points in a $\{100\}$ lattice plane, etc.; a simple hexagonal Bravais lattice is taken into itself by a rotation through 60° about a line of lattice points parallel to the c-axis, reflection in a lattice plane perpendicular to the c-axis, etc.

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[1] An example of such a relation is the orthonormality condition $\mathbf{a}_i \cdot \mathbf{a}_j = a^2\delta_{ij}$, holding for the appropriate primitive vectors in a simple cubic Bravais lattice.

[2] A detailed view of the subject can be found in M. J. Buerger, *Elementary Crystallography*, Wiley, New York, 1963.

[3] In this chapter a Bravais lattice is viewed as the crystal structure formed by placing at each point of an abstract Bravais lattice a basis of maximum possible symmetry (such as a sphere. centered on the lattice point) so that no symmetries of the point Bravais lattice are lost because of the insertion of the basis.

[4] Operations that preserve the distance between all lattice points.

[5] We shall avoid the language of mathematical group theory, since we shall make no use of the analytical conclusions to which it leads.

[6] Reflection in a plane replaces an object by its mirror image in that plane; inversion in a point P takes the point with coordinates $\mathbf{r}$ (with respect to P as origin) into $-\mathbf{r}$. All Bravais lattices have inversion symmetry in any lattice point (Problem 1).

Any symmetry operation of a Bravais lattice can be compounded out of a translation $T_{\mathbf{R}}$ through a lattice vector **R** and a rigid operation leaving at least one lattice point fixed.[7] This is not immediately obvious. A simple cubic Bravais lattice, for example, is left fixed by a rotation through 90° about a ⟨100⟩ axis that passes through the center of a cubic primitive cell with lattice points at the eight vertices of the cube. This is a rigid operation that leaves no lattice point fixed. However, it can be compounded out of a translation through a Bravais lattice vector and a rotation

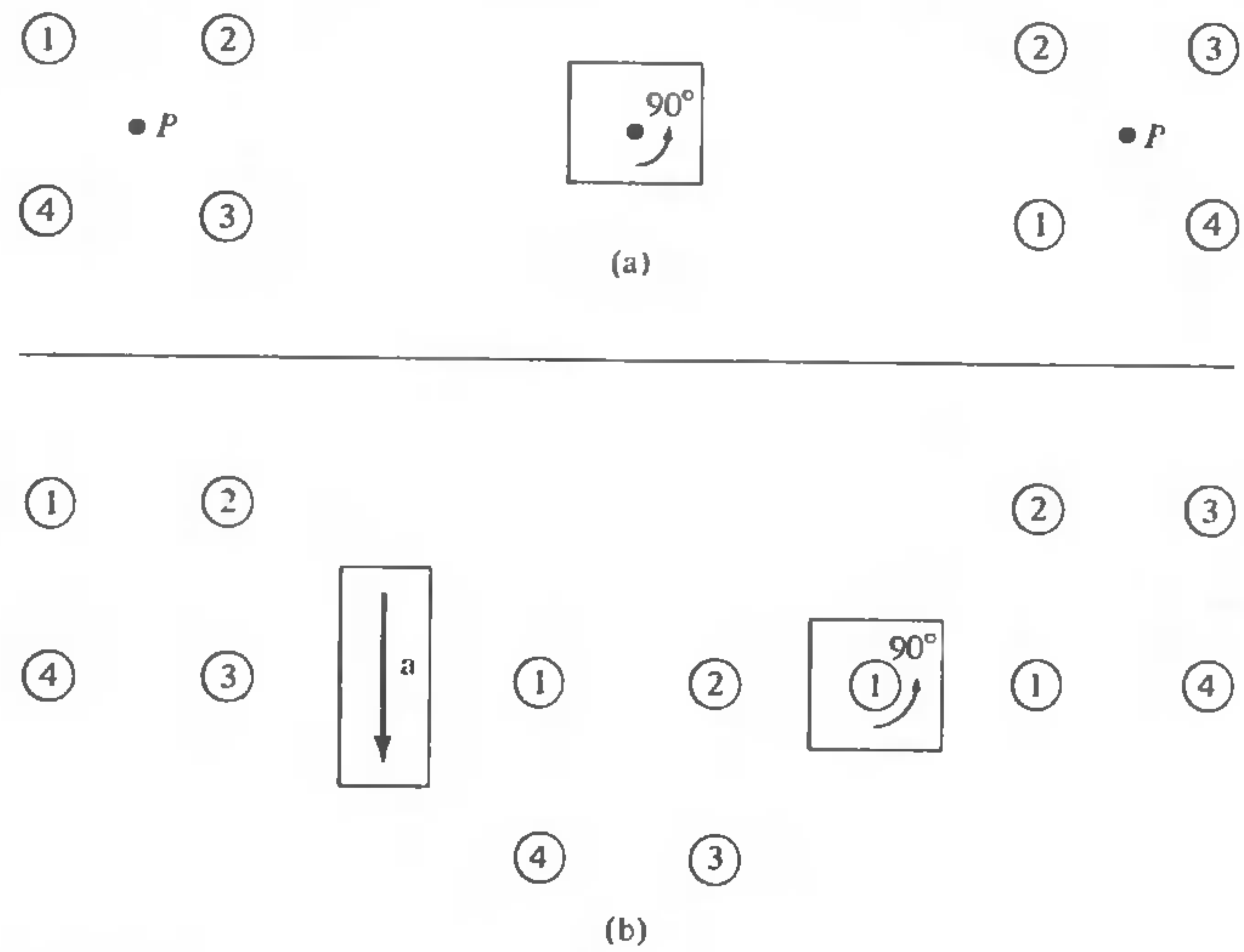

Figure 7.1
(a) A simple cubic lattice is carried into itself by a rotation through 90° about an axis that contains no lattice points. The rotation axis is perpendicular to the page, and only the four lattice points closest to the axis in a single lattice plane are shown. (b) Illustrating how the same final result can be compounded out of (at left) a translation through a lattice constant and (at right) a rotation about the lattice point numbered 1.

about a line of lattice points, as illustrated in Figure 7.1. That such a representation is always possible can be seen as follows:

Consider a symmetry operation S that leaves *no* lattice point fixed. Suppose it takes the origin of the lattice **O** into the point **R**. Consider next the operation one gets by first applying S, and then applying a translation through $-\mathbf{R}$, which we denote by $T_{-\mathbf{R}}$. The composite operation, which we call $T_{-\mathbf{R}}S$, is also a symmetry of the lattice, but it leaves the origin fixed, since S transports the origin to **R** while $T_{-\mathbf{R}}$ carries **R** back to the origin. Thus $T_{-\mathbf{R}}S$ is an operation that leaves at least one lattice point (namely the origin) fixed. If, however, after performing the operation $T_{-\mathbf{R}}S$ we then perform the operation $T_{\mathbf{R}}$, the result is equivalent to the operation S alone, since the final application of $T_{\mathbf{R}}$ just undoes the preceding application of $T_{-\mathbf{R}}$. Therefore S can be compounded out of $T_{-\mathbf{R}}S$, which leaves a point fixed, and $T_{\mathbf{R}}$, which is a pure translation.

[7] Note that translation through a lattice vector (other than **O**) leaves no point fixed.

Thus the full symmetry group of a Bravais lattice[8] contains only operations of the following form:

1. Translations through Bravais lattice vectors;
2. Operations that leave a particular point of the lattice fixed;
3. Operations that can be constructed by successive applications of the operations of type (1) or (2).

The Seven Crystal Systems

When examining nontranslational symmetries, one often considers not the entire space group of a Bravais lattice, but only those operations that leave a particular point fixed (i.e., the operations in category (2) above). This subset of the full symmetry group of the Bravais lattice is called the *point group* of the Bravais lattice.

There turn out to be only seven distinct point groups that a Bravais lattice can have.[9] Any crystal structure belongs to one of *seven crystal systems*, depending on which of these seven point groups is the point group of its underlying Bravais lattice. The seven crystal systems are enumerated in the next section.

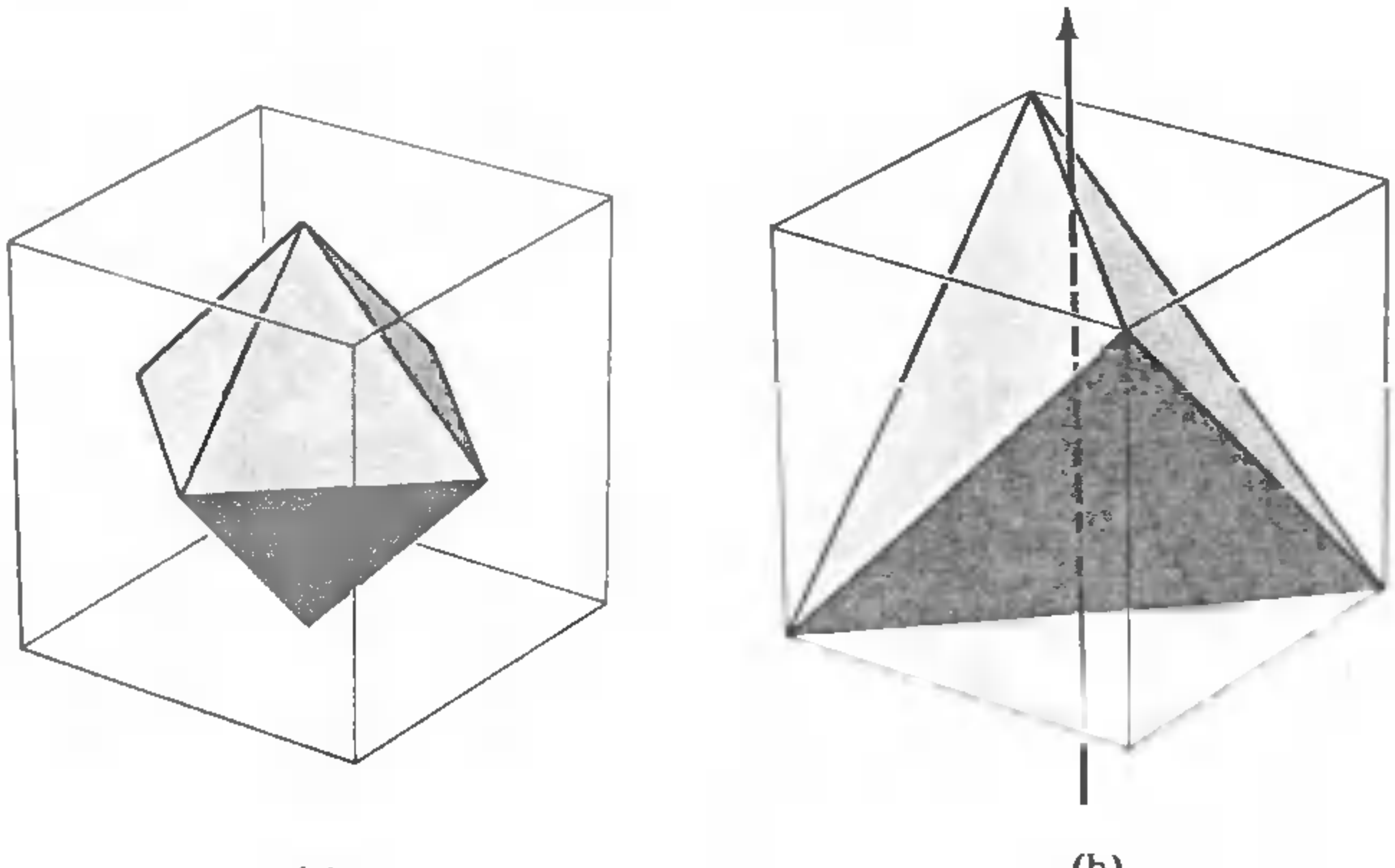

Figure 7.2
(a) Every symmetry operation of a cube is also a symmetry operation of a regular octahedron, and vice versa. Thus the cubic group is identical to the octahedral group. (b) Not every symmetry operation of a cube is a symmetry operation of a regular tetrahedron. For example, rotation through 90° about the indicated vertical axis takes the cube into itself, but not the tetrahedron.

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[8] We shall see below that a general crystal structure can have additional symmetry operations that are not of types (1), (2), or (3). They are known as "screw axes" and "glide planes."

[9] Two point groups are identical if they contain precisely the same operations. For example, the set of all symmetry operations of a cube is identical to the set of all symmetry operations of a regular octahedron, as can readily be seen by inscribing the octahedron suitably in the cube (Figure 7.2a). On the other hand, the symmetry group of the cube is not equivalent to the symmetry group of the regular tetrahedron. The cube has more symmetry operations (Figure 7.2b).

The Fourteen Bravais Lattices

When one relaxes the restriction to point operations and considers the full symmetry group of the Bravais lattice, there turn out to be fourteen distinct space groups that a Bravais lattice can have.[10] Thus, from the point of view of symmetry, there are fourteen different kinds of Bravais lattice. This enumeration was first done by M. L. Frankenheim (1842). Frankenheim miscounted, however, reporting fifteen possibilities. A. Bravais (1845) was the first to count the categories correctly.

Enumeration of the Seven Crystal Systems and Fourteen Bravais Lattices

We list below the seven crystal systems and the Bravais lattices belonging to each. The number of Bravais lattices in a system is given in parentheses after the name of the system:

***Cubic* (*3*)** The cubic system contains those Bravais lattices whose point group is just the symmetry group of a cube (Figure 7.3a). Three Bravais lattices with nonequivalent space groups all have the cubic point group. They are the *simple cubic, body-centered cubic,* and *face-centered cubic.* All three have been described in Chapter 4.

***Tetragonal* (2)** One can reduce the symmetry of a cube by pulling on two opposite faces to stretch it into a rectangular prism with a square base, but a height not equal to the sides of the square (Figure 7.3b). The symmetry group of such an object is the tetragonal group. By so stretching the simple cubic Bravais lattice one constructs the *simple tetragonal* Bravais lattice, which can be characterized as a Bravais lattice generated by three mutually perpendicular primitive vectors, only two of which are of equal length. The third axis is called the c-axis. By similarly stretching the body-centered and face-centered cubic lattices only one more Bravais lattice of the tetragonal system is constructed, the *centered tetragonal.*

To see why there is no distinction between body-centered and face-centered tetragonal, consider Figure 7.4a, which is a representation of a centered tetragonal Bravais lattice viewed along the c-axis. The points 2 lie in a lattice plane a distance

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[10] The equivalence of two Bravais lattice space groups is a somewhat more subtle notion than the equivalence of two point groups (although both reduce to the concept of "isomorphism" in abstract group theory). It is no longer enough to say that two space groups are equivalent if they have the same operations, for the operations of identical space groups can differ in inconsequential ways. For example, two simple cubic Bravais lattices with different lattice constants, a and a', are considered to have the same space groups even though the translations in one are in steps of a, whereas the translations in the other are in steps of a'. Similarly, we would like to regard all simple hexagonal Bravais lattices as having identical space groups, regardless of the value of c/a, which is clearly irrelevant to the total symmetry of the structure.

We can get around this problem by noting that in such cases one can continuously deform a structure of a given type into another of the same type without ever losing any of the symmetry operations along the way. Thus one can uniformly expand the cube axes from a to a', always maintaining the simple cubic symmetry, or one can stretch (or shrink) the c-axis (or a-axis), always maintaining the simple hexagonal symmetry. Therefore two Bravais lattices can be said to have the same space group if it is possible continuously to transform one into the other in such a way that every symmetry operation of the first is continuously transformed into a symmetry operation of the second, and there are no additional symmetry operations of the second not so obtained from symmetry operations of the first.

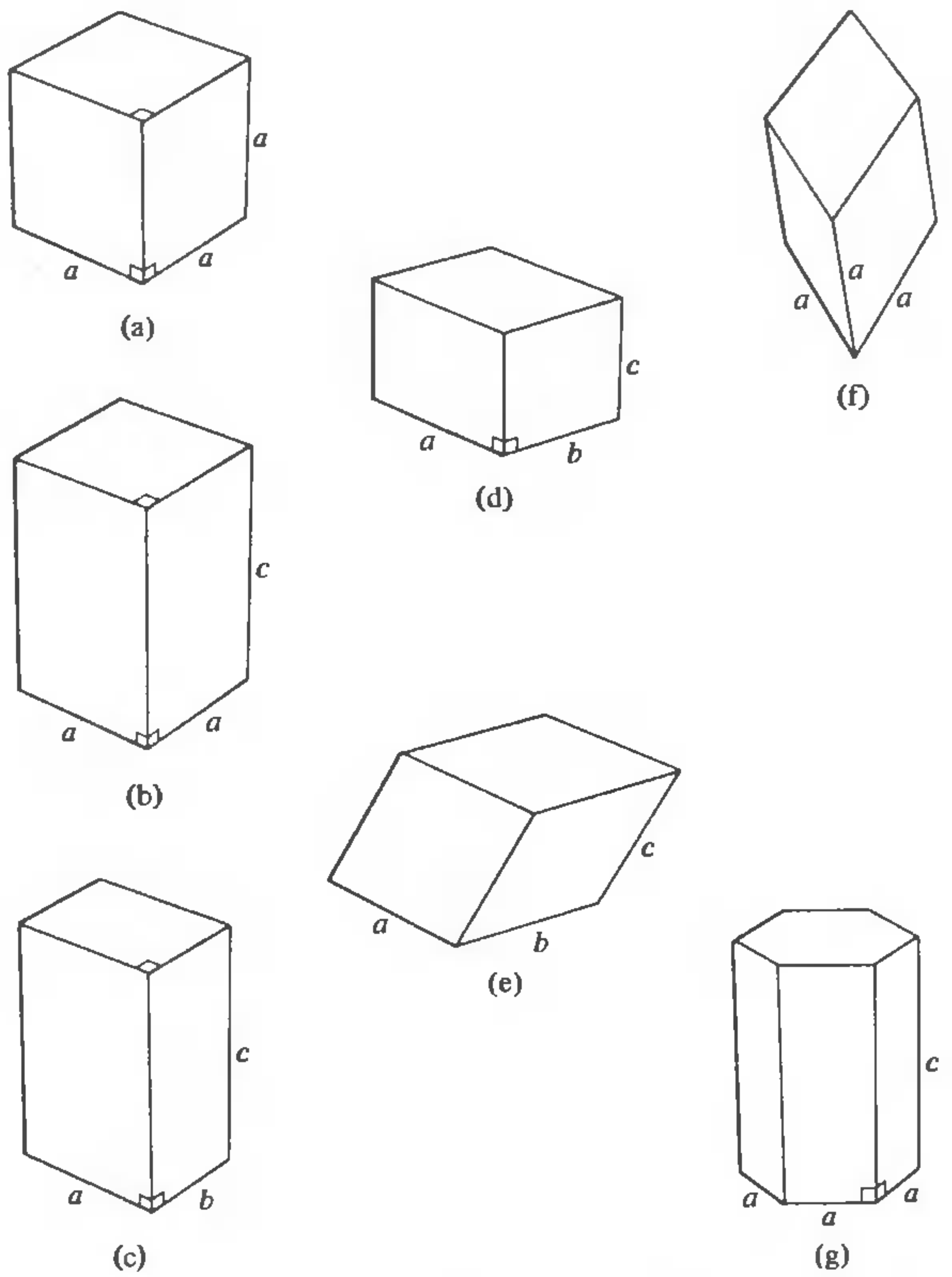
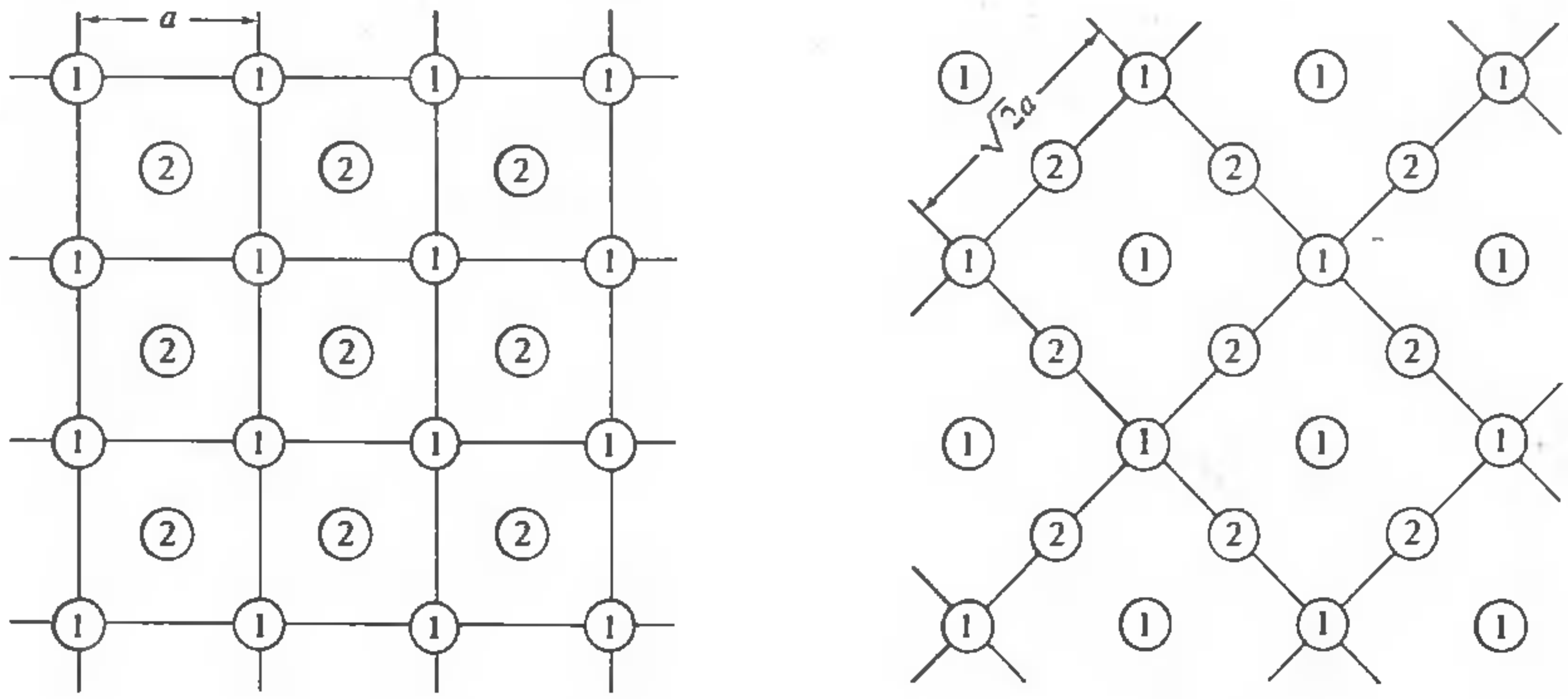


Figure 7.3
Objects whose symmetries are the point-group symmetries of Bravais lattices belonging to the seven crystal systems: (a) cubic; (b) tetragonal; (c) orthorhombic; (d) monoclinic; (e) triclinic; (f) trigonal; (g) hexagonal.

$c/2$ from the lattice plane containing the points 1. If $c = a$, the structure is nothing but a body-centered cubic Bravais lattice, and for general c it can evidently be viewed as the result of stretching the bcc lattice along the c-axis. However, precisely the same lattice can also be viewed along the c-axis, as in Figure 7.4b, with the lattice planes regarded as centered square arrays of side $a' = \sqrt{2}a$. If $c = a'/2 = a/\sqrt{2}$, the structure is nothing but a face-centered cubic Bravais lattice, and for general c it can therefore be viewed as the result of stretching the fcc lattice along the c-axis.

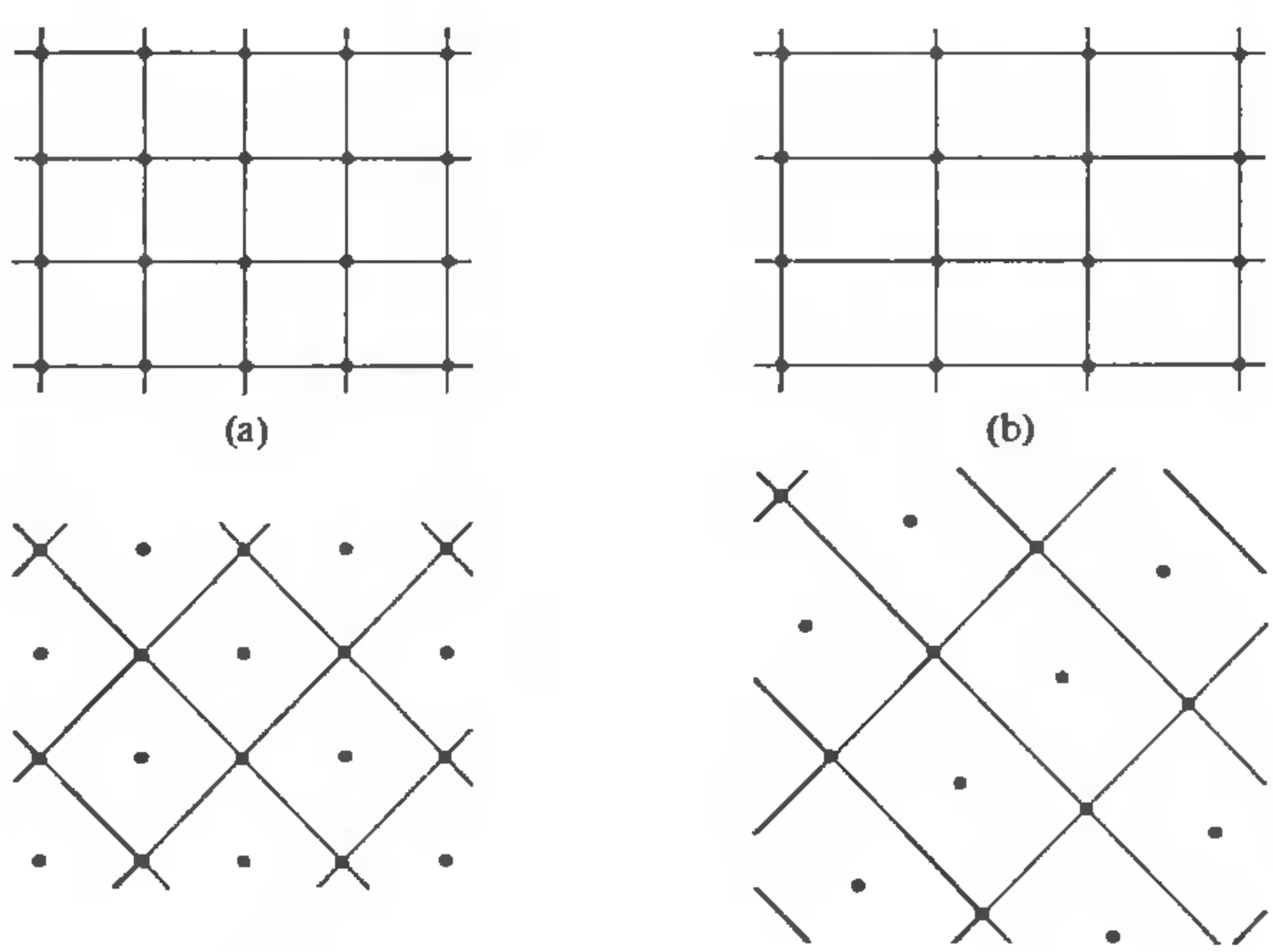
Putting it the other way around, face-centered cubic and body-centered cubic are both special cases of centered tetragonal, in which the particular value of the c/a ratio introduces extra symmetries that are revealed most clearly when one views the lattice as in Figure 7.4a (bcc) or Figure 7.4b (fcc).

***Orthorhombic* (*4*)** Continuing to still less symmetric deformations of the cube, one can reduce tetragonal symmetry by deforming the square faces of the object in Figure 7.3b into rectangles, producing an object with mutually perpendicular sides of three unequal lengths (Figure 7.3c). The orthorhombic group is the symmetry group of such an object. By stretching a simple tetragonal lattice along one of the a-axes (Figure 7.5a and b), one produces the *simple orthorhombic* Bravais lattice. However, by stretching the simple tetragonal lattice along a square diagonal (Figure 7.5c and d) one produces a second Bravais lattice of orthorhombic point group symmetry, the *base-centered* orthorhombic.



(a) (b)

Figure 7.4
Two ways of viewing the same centered tetragonal Bravais lattice. The view is along the c-axis. The points labeled 1 lie in a lattice plane perpendicular to the c-axis, and the points labeled 2 lie in a parallel lattice plane a distance $c/2$ away. In (a) the points 1 are viewed as a simple square array, stressing that centered tetragonal is a distortion of body-centered cubic. In (b) the points 1 are viewed as a centered square array, stressing that centered tetragonal is also a distortion of face-centered cubic.



(a) (b) (c) (d)

Figure 7.5
Two ways of deforming the same simple tetragonal Bravais lattice. The view is along the c-axis, and a single lattice plane is shown. In (a) bonds are drawn to emphasize that the points in the plane can be viewed as a simple square array. Stretching along a side of that array leads to the rectangular nets (b), stacked directly above one another. The resulting Bravais lattice is simple orthorhombic. In (c) lines are drawn to emphasize that the same array of points as shown in (a) can also be viewed as a centered square array. Stretching along a side of that array (i.e., along a diagonal of the square array emphasized in (a)) yields the centered rectangular nets (d), stacked directly above one another. The resul Bravais lattice is base-centered orthorhombic.

In the same way, one can reduce the point symmetry of the centered tetragonal lattice to orthorhombic in two ways, stretching either along one set of parallel lines drawn in Figure 7.4a to produce *body-centered orthorhombic*, or along one set of parallel lines in Figure 7.4b, producing *face-centered orthorhombic*.

These four Bravais lattices exhaust the orthorhombic system.

Monoclinic (*2*) One can reduce orthorhombic symmetry by distorting the rectangular faces perpendicular to the *c*-axis in Figure 7.3c into general parallelograms. The symmetry group of the resulting object (Figure 7.3d) is the monoclinic group. By so distorting the simple orthorhombic Bravais lattice one produces the *simple monoclinic* Bravais lattice, which has no symmetries other than those required by the fact that it can be generated by three primitive vectors, one of which is perpendicular to the plane of the other two. Similarly, distorting the base-centered orthorhombic Bravais lattice produces a lattice with the same simple monoclinic space group. However, so distorting either the face-centered or body-centered orthorhombic Bravais lattices produces the *centered monoclinic* Bravais lattice (Figure 7.6).

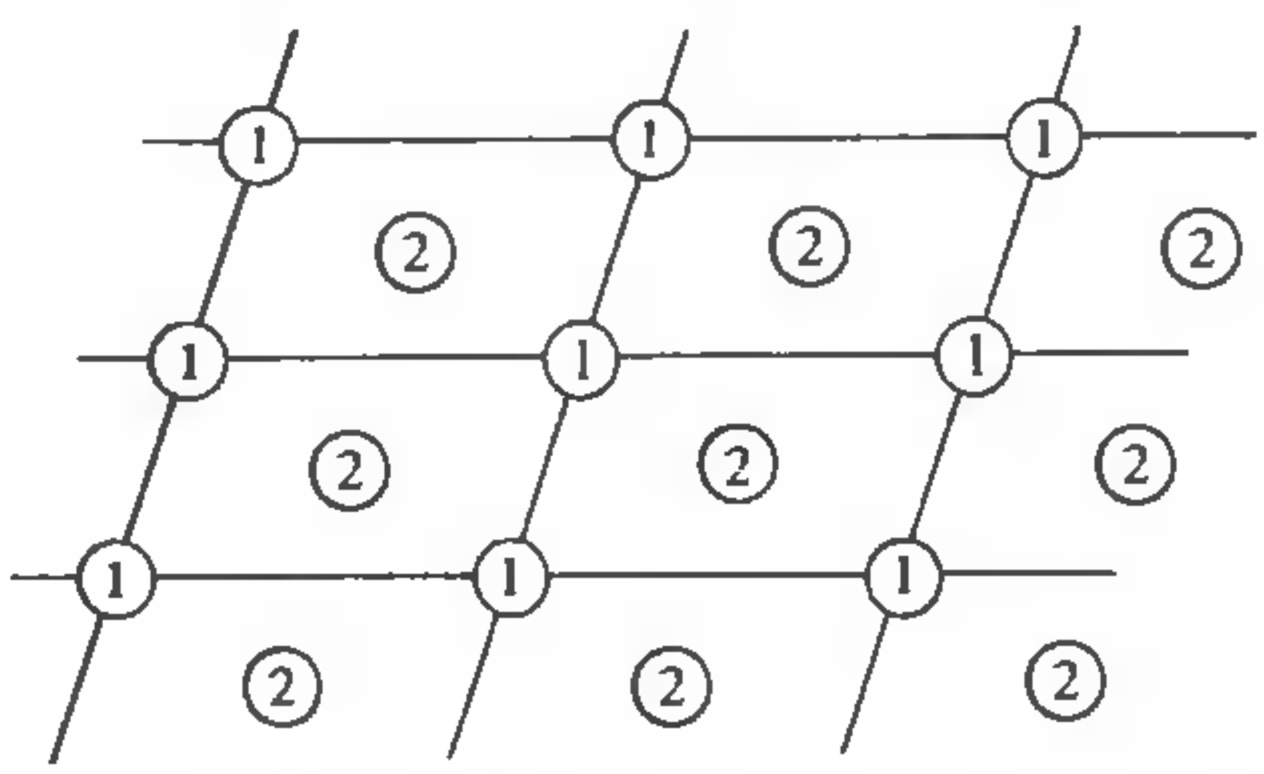


Figure 7.6
View along the *c*-axis of a centered monoclinic Bravais lattice. The points labeled 1 lie in a lattice plane perpendicular to the *c*-axis. The points labeled 2 lie in a parallel lattice plane a distance $c/2$ away, and are directly above the centers of the parallelograms formed by the points 1.

Note that the two monoclinic Bravais lattices correspond to the two tetragonal ones. The doubling in the orthorhombic case reflects the fact that a rectangular net and a centered rectangular net have distinct two-dimensional symmetry groups, while a square net and centered square net are not distinct, nor are a parallelogram net and centered parallelogram net.

Triclinic (*1*) The destruction of the cube is completed by tilting the *c*-axis in Figure 7.3d so that it is no longer perpendicular to the other two, resulting in the object pictured in Figure 7.3e, upon which there are no restrictions except that pairs of opposite faces are parallel. By so distorting either monoclinic Bravais lattice one constructs the *triclinic* Bravais lattice. This is the Bravais lattice generated by three primitive vectors with no special relationships to one another, and is therefore the Bravais lattice of minimum symmetry. The triclinic point group is not, however, the group of an object without any symmetry, since any Bravais lattice is invariant under an inversion in a lattice point. That, however, is the only symmetry required by the general definition of a Bravais lattice, and therefore the only operation[11] in the triclinic point group.

By so torturing a cube we have arrived at twelve of the fourteen Bravais lattices and five of the seven crystal systems. We can find the thirteenth and sixth by returning to the original cube and distorting it differently:

[11] Other than the identity operation (which leaves the lattice where it is), which is always counted among the members of a symmetry group.

***Trigonal* (*1*)** The trigonal point group describes the symmetry of the object one produces by stretching a cube along a body diagonal (Figure 7.3f). The lattice made by so distorting any of the three cubic Bravais lattices is the *rhombohedral* (or *trigonal*) Bravais lattice. It is generated by three primitive vectors of equal length that make equal angles with one another.[12]

Finally, unrelated to the cube, is:

***Hexagonal* (*1*)** The hexagonal point group is the symmetry group of a right prism with a regular hexagon as base (Figure 7.3g). The *simple hexagonal* Bravais lattice (described in Chapter 4) has the hexagonal point group and is the only Bravais lattice in the hexagonal system.[13]

The seven crystal systems and fourteen Bravais lattices described above exhaust the possibilities. This is far from obvious (or the lattices would have been known as Frankenheim lattices). However, it is of no practical importance to understand why these are the only distinct cases. It is enough to know why the categories exist, and what they are.

THE CRYSTALLOGRAPHIC POINT GROUPS AND SPACE GROUPS

We next describe the results of a similar analysis, applied not to Bravais lattices but to general crystal structures. We consider the structure obtained by translating an arbitrary object through the vectors of any Bravais lattice, and try to classify the symmetry groups of the arrays so obtained. These depend both on the symmetry of the object and the symmetry of the Bravais lattice. Because the objects are no longer required to have maximum (e.g., spherical) symmetry, the number of symmetry groups is greatly increased: there turn out to be 230 different symmetry groups that a lattice with a basis can have, known as the 230 *space groups*. (This is to be compared with the fourteen space groups that result when the basis is required to be completely symmetric.)

The possible point groups of a general crystal structure have also been enumerated. These describe the symmetry operations that take the crystal structure into itself while leaving one point fixed (i.e., the nontranslational symmetries). There are thirty-two distinct point groups that a crystal structure can have, known as the *thirty-two crystallographic point groups*. (This is to be compared with the seven point groups one can have when the basis is required to have full symmetry.)

These various numbers and their relations to one another are summarized in Table 7.1.

The thirty-two crystallographic point groups can be constructed out of the seven Bravais lattice point groups by systematically considering all possible ways of reducing the symmetry of the objects (Figure 7.3) characterized by these groups.

Each of the twenty-five new groups constructed in this way is associated with one

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[12] Special values of that angle may introduce extra symmetries, in which case the lattice may actually be one of the three cubic types. See, for example, Problem 2(a).

[13] If one tries to produce further Bravais lattices from distortions of the simple hexagonal, one finds that changing the angle between the two primitive vectors of equal length perpendicular to the *c*-axis yields a base-centered orthorhombic lattice, changing their magnitudes as well leads to monoclinic, and tilting the *c*-axis from the perpendicular leads, in general, to triclinic.

Table 7.1
POINT AND SPACE GROUPS OF BRAVAIS LATTICES AND CRYSTAL STRUCTURES

	BRAVAIS LATTICE (BASIS OF SPHERICAL SYMMETRY)	CRYSTAL STRUCTURE (BASIS OF ARBITRARY SYMMETRY)
Number of point groups:	7 ("the 7 crystal systems")	32 ("the 32 crystallographic point groups")
Number of space groups:	14 ("the 14 Bravais lattices")	230 ("the 230 space groups")

of the seven crystal systems according to the following rule: Any group constructed by reducing the symmetry of an object characterized by a particular crystal system continues to belong to that system until the symmetry has been reduced so far that all of the remaining symmetry operations of the object are also found in a less symmetrical crystal system; when this happens the symmetry group of the object is assigned to the less symmetrical system. Thus the crystal system of a crystallographic point group is that of the least symmetric[14] of the seven Bravais lattice point groups containing every symmetry operation of the crystallographic group.

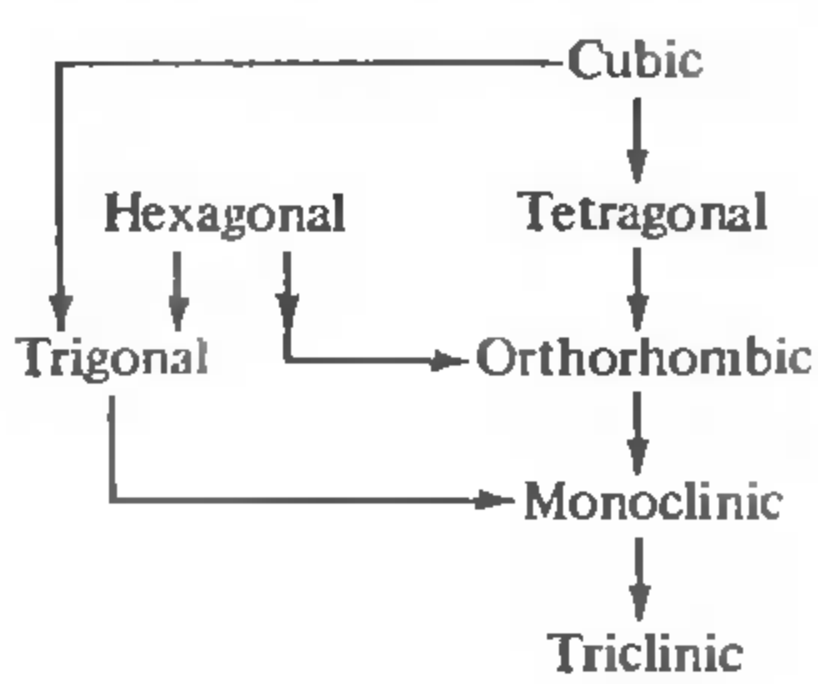


Figure 7.7
The hierarchy of symmetries among the seven crystal systems. Each Bravais lattice point group contains all those that can be reached from it by moving in the direction of the arrows.

Objects with the symmetries of the five crystallographic point groups in the cubic system are pictured in Table 7.2. Objects with the symmetries of the twenty-seven noncubic crystallographic groups are shown in Table 7.3.

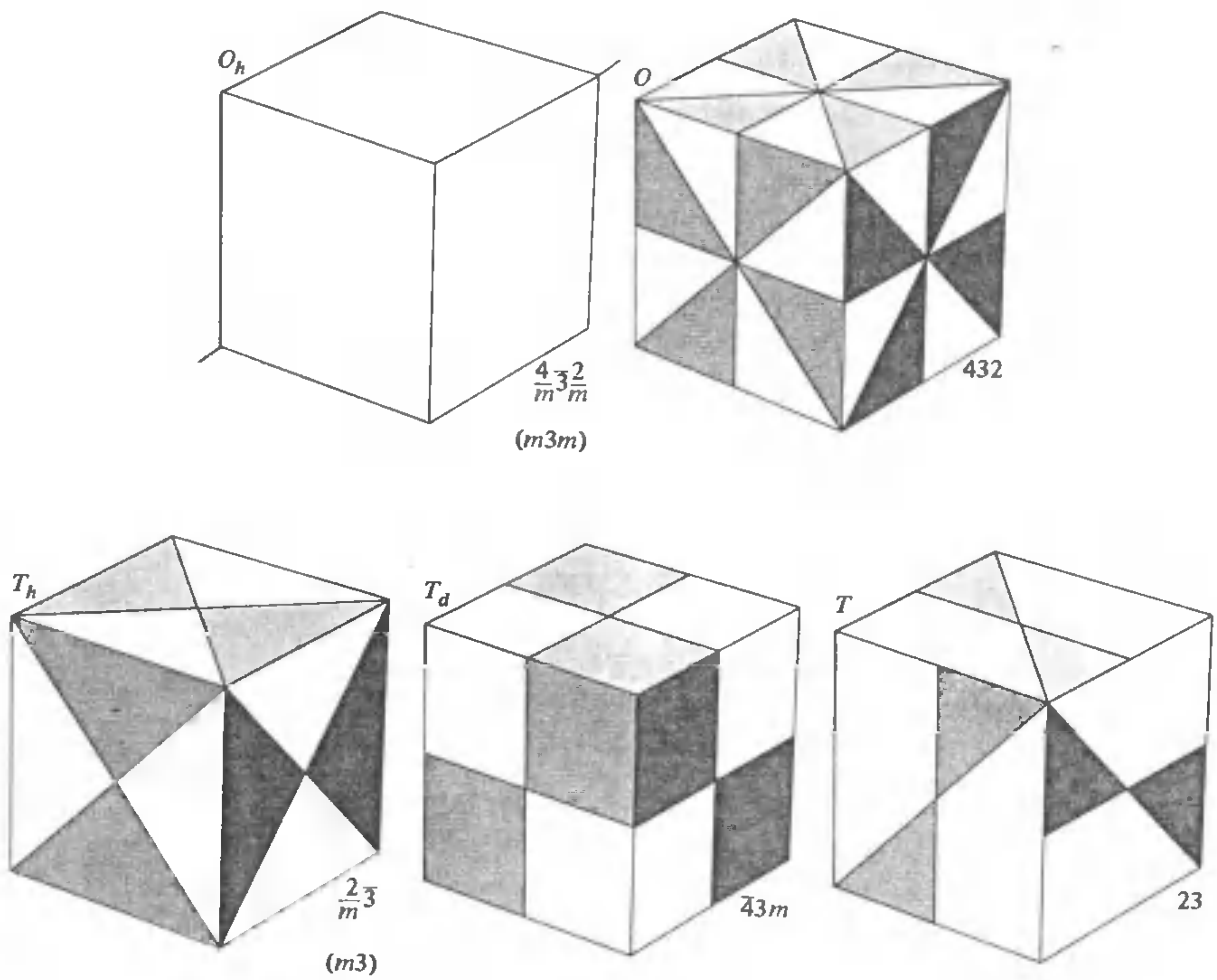
Crystallographic point groups may contain the following kinds of symmetry operations:

1. **Rotations through Integral Multiples of $2\pi/n$ about Some Axis** The axis is called an n-fold rotation axis. It is easily shown (Problem 6) that a Bravais lattice can

[14] The notion of a hierarchy of crystal system symmetries needs some elaboration. In Figure 7.7 each crystal system is more symmetric than any that can be reached from it by moving along arrows; i.e., the corresponding Bravais lattice point group has no operations that are not also in the groups from which it can be so reached. There appears to be some ambiguity in this scheme since the four pairs cubic-hexagonal, tetragonal-hexagonal, tetragonal-trigonal, and orthorhombic-trigonal are not ordered by the arrows. Thus one might imagine an object all of whose symmetry operations belonged to both the tetragonal and trigonal groups but to no group lower than both of these. The symmetry group of such an object could be said to belong to either the tetragonal or trigonal systems, since there would be no unique system of lowest symmetry. It turns out, however, both in this and the other three ambiguous cases, that all symmetry elements common to both groups in a pair also belong to a group that is lower than both in the hierarchy. (For example, any element common to both the tetragonal and the trigonal groups also belongs to the monoclinic group.) There is therefore always a unique group of lowest symmetry.

Table 7.2

OBJECTS WITH THE SYMMETRY OF THE FIVE CUBIC CRYSTALLOGRAPHIC POINT GROUPS[a]



[a] To the left of each object is the Schoenflies name of its symmetry group and to the right is the international name. The unpictured faces may be deduced from the fact that rotation about a body diagonal through 120° is a symmetry operation for all five objects. (Such an axis is shown on the undecorated cube.)

contain only 2-, 3-, 4-, or 6-fold axes. Since the crystallographic point groups are contained in the Bravais lattice point groups, they too can only have these axes.

2. **Rotation-Reflections** Even when a rotation through $2\pi/n$ is not a symmetry element, sometimes such a rotation followed by a reflection in a plane perpendicular to the axis may be. The axis is then called an n-fold rotation-reflection axis. For example, the groups S_6 and S_4 (Table 7.3) have 6- and 4-fold rotation-reflection axes.
3. **Rotation-Inversions** Similarly, sometimes a rotation through $2\pi/n$ followed by an inversion in a point lying on the rotation axis is a symmetry element, even though such a rotation by itself is not. The axis is then called an n-fold rotation-inversion axis. The axis in S_4 (Table 7.3), for example, is also a 4-fold rotation-inversion axis. However, the axis in S_6 is only a 3-fold rotation-inversion axis.
4. **Reflections** A reflection takes every point into its mirror image in a plane, known as a mirror plane.

Table 7.3
THE NONCUBIC CRYSTALLOGRAPHIC POINT GROUPS[a]

SCHOENFLIES	HEXAGONAL	TETRAGONAL	TRIGONAL	ORTHORHOMBIC	MONOCLINIC	TRICLINIC	INTERNATIONAL
C_n	C_6 6	C_4 4	C_3 3		C_2 2	C_1 1	n
C_{nv}	C_{6v} $6mm$	C_{4v} $4mm$	C_{3v} $3m$	C_{2v} $2mm$			nmm (n even) nm (n odd)
C_{nh}	C_{6h} $6/m$	C_{4h} $4/m$			C_{2h} $2/m$		n/m
	C_{3h} $\bar{6}$				C_{1h} $(\bar{2})$ m		$\bar{n}$
S_n		S_4 $\bar{4}$	S_6 (C_{3i}) $\bar{3}$			S_2 (C_i) $\bar{1}$	
D_n	D_6 622	D_4 422	D_3 32	D_2 (V) 222			$n22$ (n even) $n2$ (n odd)
D_{nh}	D_{6h} $6/mmm$	D_{4h} $4/mmm$		D_{2h} (mmm) (V_h) $2/mmm$			$\frac{n}{m}\frac{2}{m}\frac{2}{m}$ (n/mmm)
	D_{3h} $\bar{6}2m$						$\bar{n}2m$ (n even) $\bar{n}\frac{2}{m}$ (n odd)
D_{nd}		D_{2d} (V_d) $\bar{4}2m$	D_{3d} $(\bar{3}m)$ $\bar{3}\frac{2}{m}$				

[a] Table caption on p. 123.

Table 7.3 (*continued*)

The unpictured faces can be deduced by imagining the representative objects to be rotated about the n-fold axis, which is always vertical. The Schoenflies name of the group is given to the left of the representative object, and the international designation the right. The groups are organized into vertical columns by crystal system, and into horizontal rows by the Schoenflies or international type. Note that the Schoenflies categories (given on the extreme left of the table) divide up the groups somewhat differently from the international categories (given on the extreme right). In most (but not all) cases the representative objects have been made by simply decorating in the appropriate symmetry reducing manner the faces of the objects used to represent the crystal systems (Bravais lattice point groups) in Figure 7.3. Exceptions are the trigonal groups and two of the hexagonal groups, where the figures have been changed to emphasize the similarity within the (horizontal) Schoenflies categories. For a representation of the trigonal groups by decorations of the object in Figure 7.3f, see Problem 4.

5. **Inversions** An inversion has a single fixed point. If that point is taken as the origin, then every other point $\mathbf{r}$ is taken into $-\mathbf{r}$.

Point-Group Nomenclature

Two nomenclatural systems, the Schönflies and the international, are in wide use. Both designations are given in Tables 7.2 and 7.3.

Schoenflies Notation for the Noncubic Crystallographic Point Groups The Schoenflies categories are illustrated by grouping the rows in Table 7.3 according to the labels given on the left side. They are:[15]

C_n: These groups contain only an n-fold rotation axis.

C_{nv}: In addition to the n-fold axis, these groups have a mirror plane that contains the axis of rotation, plus as many additional mirror planes as the existence of the n-fold axis requires.

C_{nh}: These groups contain in addition to the n-fold axis, a single mirror plane that is perpendicular to the axis.

S_n: These groups contain only an n-fold rotation-reflection axis.

D_n: In addition to an n-fold rotation axis, these groups contain a 2-fold axis perpendicular to the n-fold axis, plus as many additional 2-fold axes as are required by the existence of the n-fold axis.

D_{nh}: These (the most symmetric of the groups) contain all the elements of D_n plus a mirror plane perpendicular to the n-fold axis.

D_{nd}: These contain the elements of D_n plus mirror planes containing the n-fold axis, which bisect the angles between the 2-fold axes.

It is instructive to verify that the objects shown in Table 7.3 do indeed have the symmetries required by their Schoenflies names.

International Notation for the Noncubic Crystallographic Point Groups The international categories are illustrated by grouping the rows in Table 7.3 according to

[15] C stands for "cyclic," D for "dihedral," and S for "Spiegel" (mirror). The subscripts h, v, and d stand for "horizontal," "vertical," and "diagonal," and refer to the placement of the mirror planes with respect to the n-fold axis, considered to be vertical. (The "diagonal" planes in D_{nd} are vertical and bisect the angles between the 2-fold axes.)

the labels given on the right side. Three categories are identical to the Schoenflies categories:

n is the same as C_n.

nmm is the same as C_{nv}. The two m's refer to two distinct types of mirror planes containing the n-fold axis. What they are is evident from the objects illustrating $6mm$, $4mm$, and $2mm$. These demonstrate that a $2j$-fold axis takes a vertical mirror plane into j mirror planes, but in addition j others automatically appear, bisecting the angles between adjacent planes in the first set. However, a $(2j + 1)$-fold axis takes a mirror plane into $2j + 1$ equivalent ones, and therefore[16] C_{3v} is only called $3m$.

$n22$ is the same as D_n. The discussion is the same as for nmm, but now perpendicular 2-fold axes are involved instead of vertical mirror planes.

The other international categories and their relation to those of Schoenflies are as follows:

n/m is the same as C_{nh}, *except* that the international system prefers to regard C_{3h} as containing a 6-fold rotation-inversion axis, making it $\bar{6}$ (see the next category). Note also that C_{1h} becomes simply m, rather than $1/m$.

$\bar{n}$ is a group with an n-fold rotation-inversion axis. This category contains C_{3h}, disguised as $\bar{6}$. It also contains S_4, which goes nicely into $\bar{4}$. However, S_6 becomes $\bar{3}$ and S_2 becomes $\bar{1}$ by virtue of the difference between rotation-reflection and rotation-inversion axes.

$\frac{n}{m}\frac{2}{m}\frac{2}{m}$, abbreviated n/mmm, is just D_{nh}, *except* that the international system prefers to regard D_{3h} as containing a 6-fold rotation-inversion axis, making it $\bar{6}2m$ (see the next category, and note the similarity to the ejection of C_{3h} from n/m into $\bar{n}$). Note also that $2/mmm$ is conventionally abbreviated further into mmm. The full-blown international title is supposed to remind one that D_{nh} can be viewed as an n-fold axis with a perpendicular mirror plane, festooned with two sets of perpendicular 2-fold axes, each with its own perpendicular mirror planes.

$\bar{n}2m$ is the same as D_{nd}, *except* that D_{3h} is included as $\bar{6}2m$. The name is intended to suggest an n-fold rotation-inversion axis with a perpendicular 2-fold axis and a vertical mirror plane. The $n = 3$ case is again exceptional, the full name being $\bar{3}\frac{2}{m}$ (abbreviated $\bar{3}m$) to emphasize the fact that in this case the vertical mirror plane is perpendicular to the 2-fold axis.

Nomenclature for the Cubic Crystallographic Point Groups The Schoenflies and international names for the five cubic groups are given in Table 7.2. O_h is the full symmetry group of the cube (or octahedron, whence the O) including improper operations,[17] which the horizontal reflection plane (h) admits. O is the cubic (or octahedral) group without improper operations. T_d is the full symmetry group of the regular tetrahedron including all improper operations, T is the group of the regular tetrahedron excluding all improper operations, and T_h is what results when an inversion is added to T.

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16 In emphasizing the differences between odd- and even-fold axes, the international system, unlike the Schoenflies, treats the 3-fold axis as a special case.

17 Any operation that takes a right-handed object into a left-handed one is called *improper*. All others are proper. Operations containing an odd number of inversions or mirrorings are improper.

The international names for the cubic groups are conveniently distinguished from those of the other crystallographic point groups by containing 3 as a second number, referring to the 3-fold axis present in all the cubic groups.

The 230 Space Groups

We shall have mercifully little to say about the 230 space groups, except to point out that the number is larger than one might have guessed. For each crystal system one can construct a crystal structure with a different space group by placing an object with the symmetries of each of the point groups of the system into each of the Bravais lattices of the system. In this way, however, we find only 61 space groups, as shown in Table 7.4.

Table 7.4
ENUMERATION OF SOME SIMPLE SPACE GROUPS

SYSTEM	NUMBER OF POINT GROUPS	NUMBER OF BRAVAIS LATTICES	PRODUCT
Cubic	5	3	15
Tetragonal	7	2	14
Orthorhombic	3	4	12
Monoclinic	3	2	6
Triclinic	2	1	2
Hexagonal	7	1	7
Trigonal	5	1	5
Totals	32	14	61

We can eke out five more by noting that an object with trigonal symmetry yields a space group not yet enumerated, when placed in a hexagonal Bravais lattice.[18]

[18] Although the trigonal point group is contained in the hexagonal point group, the trigonal Bravais lattice cannot be obtained from the simple hexagonal by an infinitesimal distortion. (This is in contrast to all other pairs of systems connected by arrows in the symmetry hierarchy of Figure 7.7.) The trigonal point group is contained in the hexagonal point group because the trigonal Bravais lattice can be viewed as simple hexagonal with a three-point basis consisting of

$$0;\quad \tfrac{1}{3}\mathbf{a}_1, \tfrac{1}{3}\mathbf{a}_2, \tfrac{1}{3}\mathbf{c};\quad \text{and}\quad \tfrac{2}{3}\mathbf{a}_1, \tfrac{2}{3}\mathbf{a}_2, \tfrac{2}{3}\mathbf{c}.$$

As a result, placing a basis with a trigonal point group into a hexagonal Bravais lattice results in a different space group from that obtained by placing the same basis into a trigonal lattice. In no other case is this so. For example, a basis with tetragonal symmetry, when placed in a simple cubic lattice, yields exactly the same space group as it would if placed in a simple tetragonal lattice (unless there happens to be a special relation between the dimensions of the object and the length of the c-axis). This is reflected physically in the fact that there are crystals that have trigonal bases in hexagonal Bravais lattices, but none with tetragonal bases in cubic Bravais lattices. In the latter case there would be nothing in the structure of such an object to require the c-axis to have the same length as the a-axes; if the lattice did remain cubic it would be a mere coincidence. In contrast, a simple hexagonal Bravais lattice cannot distort continuously into a trigonal one, and can therefore be held in its simple hexagonal form even by a basis with only trigonal symmetry.

Because trigonal point groups can characterize a crystal structure with a hexagonal Bravais lattice, crystallographers sometimes maintain that there are only six crystal systems. This is because crystallography emphasizes the point symmetry rather than the translational symmetry. From the point of view of the Bravais lattice point groups, however, there are unquestionably seven crystal systems: the point groups D_{3d} and D_{6h} are both the point groups of Bravais lattices, and are not equivalent.

Another seven arise from cases in which an object with the symmetry of a given point group can be oriented in more than one way in a given Bravais lattice so that more than one space group arises. These 73 space groups are called *symmorphic.*

The majority of the space groups are *nonsymmorphic*, containing additional operations that cannot be simply compounded out of Bravais lattice translations and point-group operations. For there to be such additional operations it is essential that there be some special relation between the dimensions of the basis and the dimensions of the Bravais lattice. When the basis does have a size suitably matched to the primitive vectors of the lattice, two new types of operations may arise:

1. **Screw Axes** A crystal structure with a screw axis is brought into coincidence with itself by translation through a vector not in the Bravais lattice, followed by a rotation about the axis defined by the translation.
2. **Glide Planes** A crystal structure with a glide plane is brought into coincidence with itself by translation through a vector not in the Bravais lattice, followed by a reflection in a plane containing that vector.

The hexagonal close-packed structure offers examples of both types of operation, as shown in Figure 7.8. They occur only because the separation of the two basis points along the c-axis is precisely half the distance between lattice planes.

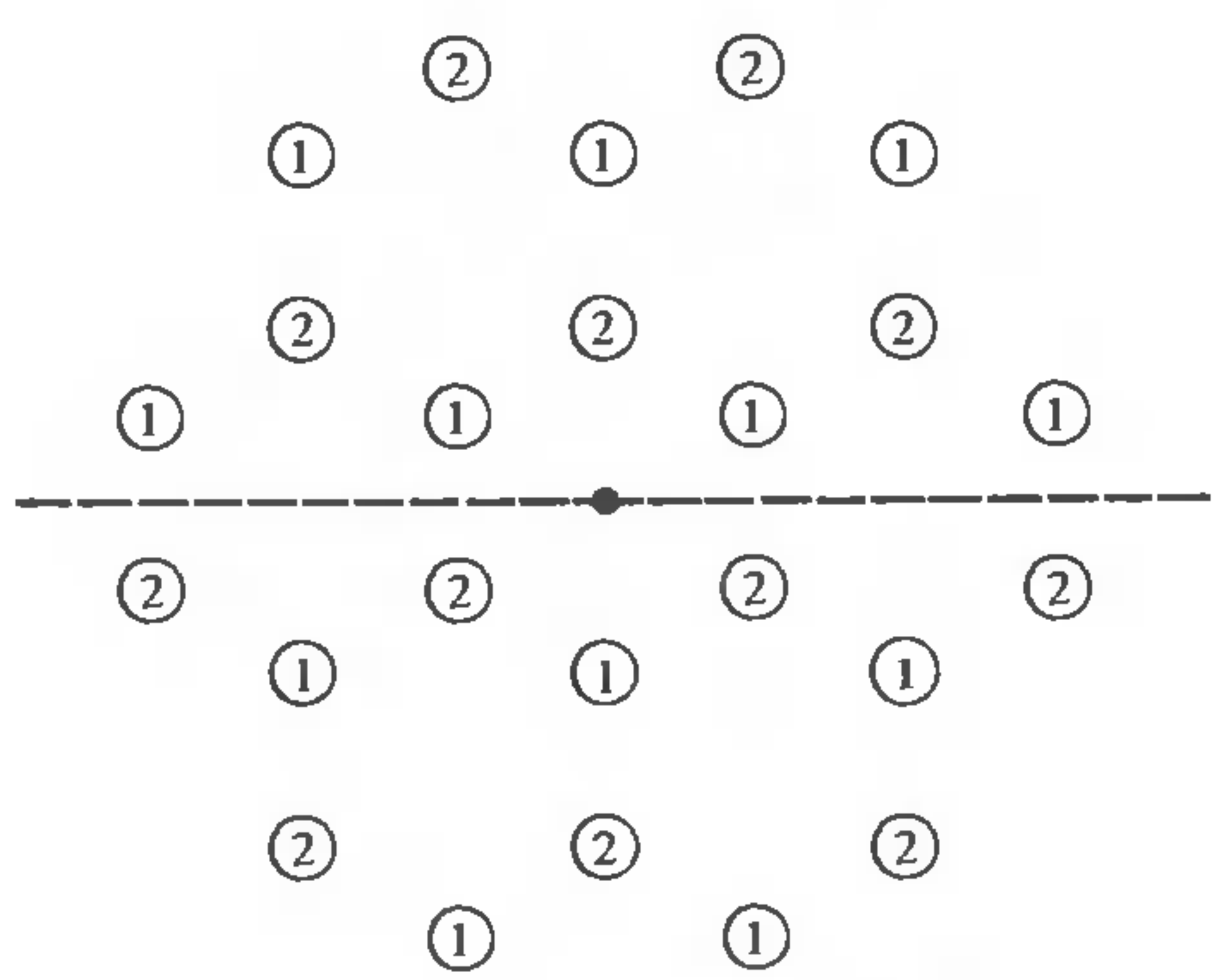

Figure 7.8
The hexagonal close-packed structure viewed along the c-axis. Lattice planes perpendicular to the c-axis are separated by $c/2$ and contain, alternately, points of type 1 and points of type 2. The line parallel to the c-axis passing through the dot in the center of the figure is a screw axis: the structure is invariant under a translation through $c/2$ along the axis followed by a rotation of 60° (but it is not invariant under either the translation or rotation alone.) The plane parallel to the c-axis that intersects the figure in the dashed line is a glide plane: the structure is invariant under a translation through $c/2$ along the c-axis followed by a reflection in the glide plane (but is not invariant under either the translation or reflection alone).

There are both Schoenflies and international systems of space-group nomenclature, which can be found, on the few occasions they may be needed, in the book by Buerger cited in footnote 2.

EXAMPLES AMONG THE ELEMENTS

In Chapter 4 we listed those elements with face-centered cubic, body-centered cubic, hexagonal close-packed, or diamond crystal structures. Over 70 percent of the elements fall into these four categories. The remaining ones are scattered among a variety of crystal structures, most with polyatomic primitive cells that are sometimes quite complex. We conclude this chapter with a few further examples listed in Table 7.5, 7.6, and 7.7. Data are from Wyckoff (cited on page 70) and are for room temperature and normal atmospheric pressure, unless stated otherwise.

Table 7.5
ELEMENTS WITH RHOMBOHEDRAL (TRIGONAL) BRAVAIS LATTICES[a]

ELEMENT	a (Å)	θ	ATOMS IN PRIMITIVE CELL	BASIS
Hg (5 K)	2.99	70°45′	1	$x = 0$
As	4.13	54°10′	2	$x = \pm 0.226$
Sb	4.51	57°6′	2	$x = \pm 0.233$
Bi	4.75	57°14′	2	$x = \pm 0.237$
Sm	9.00	23°13′	3	$x = 0, \pm 0.222$

[a] The common length of the primitive vectors is a, and the angle between any two of them is θ. In all cases the basis points expressed in terms of these primitive vectors have the form $x(\mathbf{a}_1 + \mathbf{a}_2 + \mathbf{a}_3)$. Note (Problem 2(b)) that arsenic, antimony, and bismuth are quite close to a simple cubic lattice, distorted along a body diagonal.

Table 7.6
ELEMENTS WITH TETRAGONAL BRAVAIS LATTICES[a]

ELEMENT	a (Å)	c (Å)	BASIS
In	4.59	4.94	At face-centered positions of the conventional cell
Sn (white)	5.82	3.17	At 000, $0\frac{1}{2}\frac{1}{4}$, $\frac{1}{2}0\frac{3}{4}$, $\frac{1}{2}\frac{1}{2}\frac{1}{2}$, with respect to the axes of the conventional cell

[a] The common length of two perpendicular primitive vectors is a, and the length of the third, perpendicular to these, is c. Both examples have centered tetragonal Bravais lattices, indium with a one-atom and white tin with a two-atom basis. However, both are more commonly described as simple tetragonal with bases. The conventional cell for indium is chosen to stress that it is a slightly distorted (along a cube edge) fcc structure. The white tin structure can be viewed as a diamond structure compressed along one of the cube axes.

Table 7.7
ELEMENTS WITH ORTHORHOMBIC BRAVAIS LATTICES[a]

ELEMENT	a (Å)	b (Å)	c (Å)
Ga	4.511	4.517	7.645
P (black)	3.31	4.38	10.50
Cl (113 K)	6.24	8.26	4.48
Br (123 K)	6.67	8.72	4.48
I	7.27	9.79	4.79
S (rhombic)	10.47	12.87	24.49

[a] The lengths of the three mutually perpendicular primitive vectors are a, b, and c. The structure of rhombic sulfur is complex, with 128 atoms per unit cell. The others can be described in terms of an eight-atom unit cell. For details the reader is referred to Wyckoff.

PROBLEMS

1. (a) Prove that any Bravais lattice has inversion symmetry in a lattice point. (*Hint:* Express the lattice translations as linear combinations of primitive vectors with integral coefficients.)

(b) Prove that the diamond structure is invariant under an inversion in the midpoint of any nearest neighbor bond.

2. (a) If three primitive vectors for a trigonal Bravais lattice are at angles of 90° to one another, the lattice obviously has more than trigonal symmetry, being simple cubic. Show that if the angles are 60° or arc cos $(-\frac{1}{3})$ the lattice again has more than trigonal symmetry, being face-centered cubic or body-centered cubic.

(b) Show that the simple cubic lattice can be represented as a trigonal lattice with primitive vectors $\mathbf{a}_i$ at 60° angles to one another, with a two-point basis $\pm\frac{1}{4}(\mathbf{a}_1 + \mathbf{a}_2 + \mathbf{a}_3)$. (Compare these numbers with the crystal structures in Table 7.5.)

(c) What structure results if the basis in the same trigonal lattice is taken to be $\pm\frac{1}{8}(\mathbf{a}_1 + \mathbf{a}_2 + \mathbf{a}_3)$?

3. If two systems are connected by arrows in the symmetry hierarchy of Figure 7.7, then a Bravais lattice in the more symmetric system can be reduced to one of lower symmetry by an infinitesimal distortion, except for the pair hexagonal-trigonal. The appropriate distortions have been fully described in the text in all cases except hexagonal-orthorhombic and trigonal-monoclinic.

(a) Describe an infinitesimal distortion that reduces a simple hexagonal Bravais lattice to one in the orthorhombic system.

(b) What kind of orthorhombic Bravais lattice can be reached in this way?

(c) Describe an infinitesimal distortion that reduces a trigonal Bravais lattice to one in the monoclinic system.

(d) What kind of monoclinic Bravais lattice can be reached in this way?

4. (a) Which of the trigonal point groups described in Table 7.3 is the point group of the Bravais lattice? That is, which of the representative objects has the symmetry of the object shown in Figure 7.3f?

(b) In Figure 7.9 the faces of the object of Figure 7.3f are decorated in various symmetry-reducing ways to produce objects with the symmetries of the remaining four trigonal point groups. Referring to Table 7.3, indicate the point-group symmetry of each object.

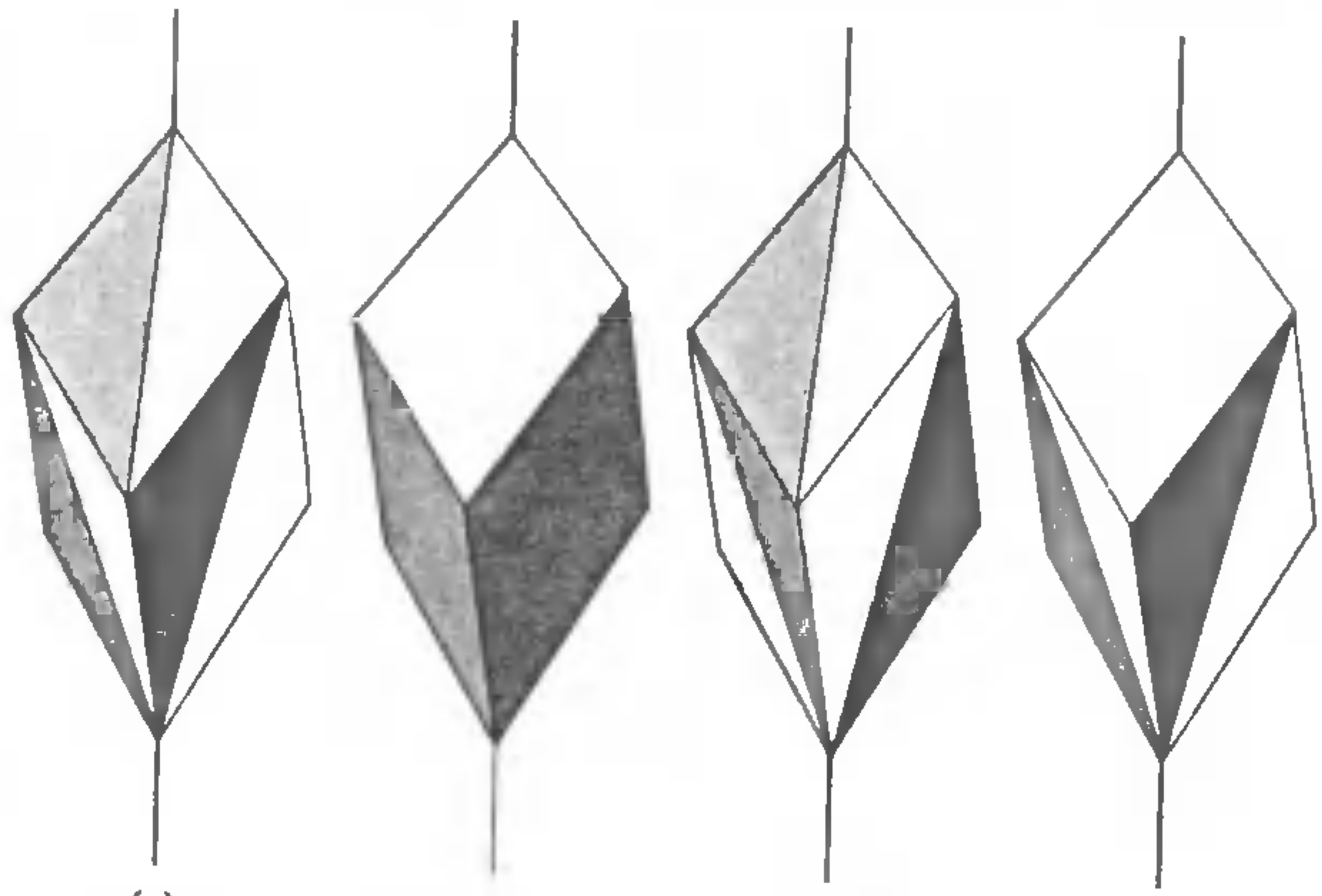

Figure 7.9
Objects with the symmetries of the trigonal groups of lower symmetry. Which is which?

5. Which of the 14 Bravais lattices other than face-centered cubic and body-centered cubic do not have reciprocal lattices of the same kind?

6. (a) Show that there is a family of lattice planes perpendicular to any n-fold rotation axis of a Bravais lattice, $n \geqslant 3$. (The result is also true when $n = 2$, but requires a somewhat more elaborate argument (Problem 7).)

(b) Deduce from (a) that an n-fold axis cannot exist in any three-dimensional Bravais lattice unless it can exist in some two-dimensional Bravais lattice.

(c) Prove that no two-dimensional Bravais lattice can have an n-fold axis with $n = 5$ or $n \geqslant 7$. (*Hint:* First show that the axis can be chosen to pass through a lattice point. Then argue by *reductio ad absurdum*, using the set of points into which the nearest neighbor of the fixed point is taken by the n rotations to find a pair of points closer together than the assumed nearest neighbor distance. (Note that the case $n = 5$ requires slightly different treatment from the others).)

7. (a) Show that if a Bravais lattice has a mirror plane, then there is a family of lattice planes parallel to the mirror plane. (*Hint:* Show from the argument on page 113 that the existence of a mirror plane implies the existence of a mirror plane containing a lattice point. It is then enough to prove that that plane contains two other lattice points not collinear with the first.)

(b) Show that if a Bravais lattice has a 2-fold rotation axis then there is a family of lattice planes perpendicular to the axis.