Symmetry Groups

Symmetry is a fundamental organizational concept in art as well as science. To develop and exploit this concept to its fullest, it must be given a precise mathematical formulation. This has been a primary motivation for developing the branch of mathematics known as "group theory." There are many kinds of symmetry, but the symmetries of rigid bodies are the most important and useful, because they are the most ubiquitous as well as the most obvious. Moreover, they provide an excellent model for the investigation of other symmetries. We have already developed the mathematical apparatus needed to describe and classify all possible rigid body symmetries. The aim of this section is to show how such a description and classification can be carried out efficiently with geometric algebra. The results have extensive applications in the theory of molecular and crystalline structure.

We say that a geometrical figure or a rigid body is "symmetrical" if there exists isometries which permute its parts while leaving the object as a whole unchanged. An isometry of this kind is called a *symmetry*. The symmetries of a given object form a group called the *symmetry group* of the object. Obviously, every symmetry group is a subgroup of the group of all isometries, the improper Euclidean group. We know, therefore, from Sec. 5.4 that any symmetry $\mathcal{S}$ of a rigid body can be given the mathematical form

$$\mathcal{S}\mathbf{x} = \{R|t\}\,\mathbf{x} = \widetilde{R}\,\mathbf{x}R + t\,, \tag{1}$$

where $\mathbf{x}$ is the position of any particle in the rigid body. This reduces the problem of describing and classifying symmetry groups to the problem of determining relations among the spinors and translation vectors for the symmetries in each group. As we shall see, this problem has a simple and elegant solution.

As usual in mathematical and physical problems, the best strategy is to study the simplest cases first, and therefrom discover results which are needed to handle the most complex cases. So let us begin by examining the 2-dimensional symmetry groups with a fixed point. The fixed point condition eliminates translations, so all the symmetries are orthogonal transformations. Consider, for example, the benzene molecule shown in Fig. 1. This molecule has the structure of a *regular hexagon* with a carbon atom at each vertex. Evidently, the simplest symmetry of this molecule is the rotation $\mathcal{R}$ taking each vertex $\mathbf{x}_k$ into its neighbor $\mathbf{x}_{k+1}$ as described by

$$\mathbf{x}_{k+1} = \mathcal{R}\mathbf{x}_k = R^\dagger\,\mathbf{x}_k R = \mathbf{x}_k R^2\,. \tag{2}$$

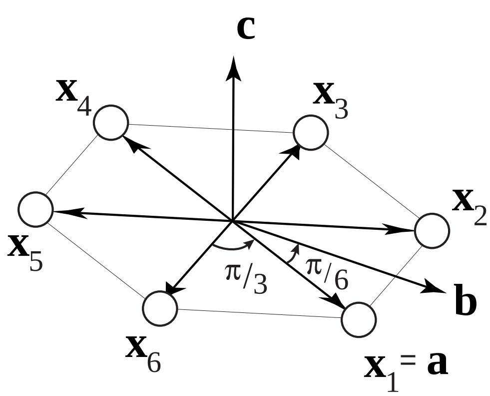


Fig. 1. Planar benzene (C_6H_6), showing generators of the symmetry group. (Hydrogen atoms not shown.)

A sixfold repetition of this rotation brings each vertex back to its original position so $\mathcal{R}$ satisfies the operator equation

$$\mathcal{R}^6 = 1\,. \tag{3}$$

This relation implies that the "powers" of $\mathcal{R}$ compose a group with six distinct elements $\mathcal{R}$, $\mathcal{R}^2$, $\mathcal{R}^3$, $\mathcal{R}^4$, $\mathcal{R}^5$, $\mathcal{R}^6 = 1$. This group, the rotational symmetry group of a hexagon, or any group isomorphic to it, is called a (or the) *cyclic group of order* 6 and commonly denoted by $\mathcal{C}_6$.

The group $\mathcal{C}_6$ is a *finite group*, so-called because it has a finite number of elements. The *order* of a finite group is the number of elements it contains. The element $\mathcal{R}$ is said to be a *generator* of $\mathcal{C}_6$, because the entire group can be generated from $\mathcal{R}$ by the group operation. The group $\mathcal{C}_6$ is completely determined by the condition $\mathcal{R}^6 = 1$ on its generator, with the tacit understanding that lower powers of $\mathcal{R}$ are not equal to the identity element. Any such condition on the generators of a group is called a *relation* of the group. A set of relations which completely determine a group is called a *presentation* of the group. For $\mathcal{C}_6$ the presentation consists of the single relation $\mathcal{R}^6 = 1$.

From preceding sections we know that it is computationally advantageous to represent rotations by spinors rather than linear operators, so we look for a representation of $\mathcal{C}_6$ by spinors. According to (2), the operator $\mathcal{R}$ corresponds to a unique spinor $S = R^2$, so the operator relation $\mathcal{R}^6 = 1$ corresponds to the spinor relation

$$S^6 = 1\,. \tag{4}$$

This presentation of $\mathcal{C}_6$ has the advantage of admitting the explicit solution

$$S = e^{2\pi\mathbf{i}/6} = e^{\mathbf{i}\pi/3}\,, \tag{5}$$

where $\mathbf{i}$ is the bivector for the plane of rotation. The representation (5) shows explicitly that the generator of $\mathcal{C}_6$ is a rotation through the angle $\pi/3 = 60°$.

Now, we know that to every rotation there corresponds two spinors differing only by a sign. Consequently, to every finite rotation group there corresponds a spinor group with twice as many elements. In the present case the generator R of the spinor group is related to the generator S of the cyclic group by $S = R^2$. Taking the negative square root of the relation $S^6 = (R^2)^6 = (R^6)^2 = 1$, we get the new relation

$$R^6 = -1\,. \tag{6}$$

This is the presentation for the *dicyclic group* of order 12 generated by R. Strictly speaking, we should include the relation $(-1)^2 = 1$ in the presentation of the group since it is not one of the group properties. However, this is taken care of by the understanding that the group elements are spinors. Since the dicyclic group presented by (6) is the spinor group of $\mathcal{C}_6$, let us denote it by $2\mathcal{C}_6$. The dicyclic group actually provides a more complete description of rotational symmetries than the cyclic group, because as we have observed in Sec. 5–3, the pair of spinors $\pm R$ distinguish equivalent rotations of opposite senses. The cyclic group does not assign a sense to rotations. This important fact is illustrated in Fig. 2 and explained more fully below.

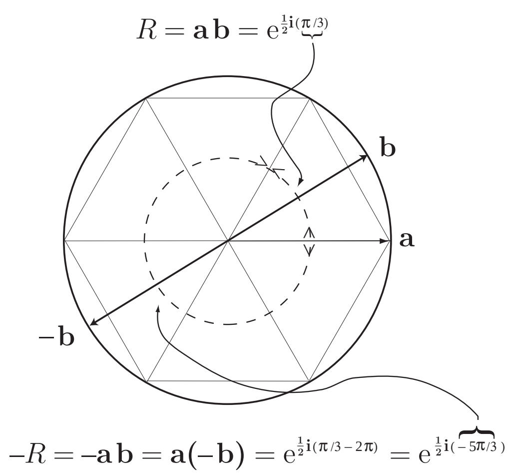


Fig. 2. Illustrating the interpretation of the spinors $\pm R = \pm\mathbf{ab} = \mathbf{a}(\pm\mathbf{b})$ as equivalent rotations with opposite sense generated by reflections with different senses.

We have seen how the rotational symmetries of a hexagon can be characterized by the single equation $S^6 = 1$ or better by $R^6 = -1$. However, a hexagon has reflectional as well as rotational symmetries. From an examination of Fig. 1, it is evident that the hexagon is invariant under reflection along any diagonal through a vertex or the midpoint of a side. For example, with $\mathbf{a} = \mathbf{x}_1$, the reflection

$$\mathcal{A}\mathbf{x} = -\mathbf{a}^{-1}\mathbf{x}\mathbf{a}\,, \tag{7}$$

is a symmetry of Fig. 1, as is the reflection

$$\mathcal{B}\mathbf{x} = -\mathbf{b}^{-1}\mathbf{x}\mathbf{b}\,, \tag{8}$$

where $\mathbf{b}$ is directed towards the midpoint of a side adjacent to the vertex, is shown in Fig. 1. These reflections generate a symmetry group of the hexagon which, for the time being, we denote by $\mathcal{H}_6$. This group is sometimes called the "dihedral group" of order 12, but that name will be reserved for a geometrically different group isomorphic to it. To avoid introducing a new name, let us be content with the symbol $\mathcal{H}_6$. Now, to get on with the study of $\mathcal{H}_6$, note that the product

$$\mathcal{B}\mathcal{A}\mathbf{x} = (\mathbf{a}\mathbf{b})^{-1}\mathbf{x}(\mathbf{a}\mathbf{b}) \tag{9}$$

is a rotation; in fact, it is the rotation $\mathcal{R}$ which generates $\mathcal{C}_6$. Therefore, $\mathcal{C}_6$ is a subgroup of $\mathcal{H}_6$. From this we can conclude that the operator equations

$$\mathcal{A}^2 = \mathcal{B}^2 = (\mathcal{A}\mathcal{B})^6 = 1 \tag{10}$$

provide an abstract presentation of $\mathcal{H}_6$.

The spinor group $2\mathcal{H}_6$ corresponding to $\mathcal{H}_6$ is generated by the vectors $\mathbf{a}$ and $\mathbf{b}$ normalized to unity, Since $R = \mathbf{a}\mathbf{b}$ must satisfy (6), the presentation of

6 distinct rotations with "positive sense" represented by	6 distinct rotations with "negative sense" represented by
$1 = \mathbf{a}^2 = \mathbf{b}^2$	$-1 = (\mathbf{a}\mathbf{b})^6 = (\mathbf{b}\mathbf{a})^6$
$\mathbf{a}\mathbf{b}$	$-\mathbf{a}\mathbf{b} = \mathbf{a}\mathbf{b}(\mathbf{b}\mathbf{a})^6 = (\mathbf{b}\mathbf{a})^5$
$(\mathbf{a}\mathbf{b})^2$	$-(\mathbf{a}\mathbf{b})^2 = (\mathbf{b}\mathbf{a})^4$
$(\mathbf{a}\mathbf{b})^3$	$-(\mathbf{a}\mathbf{b})^3 = (\mathbf{b}\mathbf{a})^3$
$(\mathbf{a}\mathbf{b})^4$	$-(\mathbf{a}\mathbf{b})^4 = (\mathbf{b}\mathbf{a})^2$
$(\mathbf{a}\mathbf{b})^5$	$-(\mathbf{a}\mathbf{b})^5 = \mathbf{b}\mathbf{a}$

12 distinct directed reflections:

$$\pm\mathbf{a},\ \pm\mathbf{aba}, \pm\mathbf{ababa} = \pm\mathbf{a}(\mathbf{ba})^2\,,$$

$$\pm\mathbf{b},\ \pm\mathbf{bab}, \pm\mathbf{babab} = \pm\mathbf{b}(\mathbf{ab})^2\,.$$

Table 1 Exhibiting the 24 distinct elements of the group $2\mathcal{H}_6$.

$2\mathcal{H}_6$ is the set of relations

$$\mathbf{a}^2 = \mathbf{b}^2 = 1\,, \tag{11}$$

$$(\mathbf{a}\mathbf{b})^6 = -1\,. \tag{12}$$

According to (8), the two vectors $\pm\mathbf{b}$ in $2\mathcal{H}_6$ correspond to the single reflection $\mathcal{B}$. Physically, however, it is possible to distinguish two distinct mirror reflections in a given plane by imagining the plane surface silvered on one side or the other. Thus, we have two distinct reflecting planes (or mirrors) with opposite orientations distinguished by the signs on their normal vectors $\pm\mathbf{b}$. An *oriented reflection* in one of these oriented (silvered) planes maintains the physical distinction between an object and its reflected image. So the two oriented reflections specified by $\pm\mathbf{b}$, describe the two possible placements of an object on opposite sides of the reflecting plane. The (unoriented) reflection $\mathcal{B}$ in (8) makes no distinction between objects and reflected images. The notion of oriented reflection is consistent with the notion of oriented rotation. For the products of oriented reflections designated by $\pm\mathbf{b}$ with an oriented reflection designated by the vector $\mathbf{a}$ will produce the spinors representing equivalent rotations with opposite senses, as illustrated in Fig. 2. Thus, each element of $2\mathcal{H}_6$ characterizes some oriented symmetry of a hexagon.

The group $2\mathcal{H}_6$ is the multiplicative group generated by two vectors $\mathbf{a}$, $\mathbf{b}$ with the properties (11, 12). The 24 distinct elements in the group are exhibited in Table 1. Note that the geometrical interpretation given to $\mathbf{a}\mathbf{b}$ in Fig. 2 permits the assignment of a definite sense to the unit spinor 1, as indicated in Table 1. So the spinor $1 = e^{\frac{1}{2}\mathbf{i}0}$ represents a rotation of zero angle in the positive sense, while the spinor $-1 = e^{-\mathbf{i}\pi} = e^{\frac{1}{2}\mathbf{i}(-2\pi)}$ represents a rotation of 2π with the opposite sense.

Ordinarily, the group $\mathcal{H}_6$ is regarded as the symmetry group of a regular hexagon. But we have seen that the corresponding spinor group $2\mathcal{H}_6$ provides a more subtle and complete characterization of the symmetries. Since the two groups are so closely related, it matters little which one is regarded as the "true" symmetry group of the hexagon. The spinor group, however, is easier to describe and work with mathematically. Consequently, as we shall see, it will be easier to generalize and relate to other symmetry groups.

Our results for the hexagon generalize immediately to any regular polygon and enable us to find and describe all the fixed point symmetry groups of all two-dimensional figures. We merely consider the multiplicative group $2\mathcal{H}_p$ generated by two *unit vectors* $\mathbf{a}$ and $\mathbf{b}$ related by the *dicyclic condition*

$$(\mathbf{a}\mathbf{b})^p = -1\,, \tag{13}$$

where p is a positive integer. The vectors $\mathbf{a}$ and $\mathbf{b}$ determine reflections (7, 8) which generate the reflection group $\mathcal{H}$. The dicyclic group $2\mathcal{C}_p$ is a subgroup of

$2\mathcal{H}_p$ generated by

$$\mathbf{ab} = e^{\mathbf{i}\pi/p} = e^{\frac{1}{2}\mathbf{i}(2\pi/p)} \tag{14}$$

the spinor for a rotation through an angle of magnitude $2\pi/p$. The corresponding rotation generates the cyclic group $\mathcal{C}_p$.

The spinor group $2\mathcal{H}_p$ or, if you will, the reflection group $\mathcal{H}_p$ is the symmetry group of a regular polygon with p sides. The group is well defined even for $p = 2$, though a two sided polygon is hard to imagine. When $p = 1$, (14) implies that $\mathbf{b} = -\mathbf{a}$, so $2\mathcal{H}_1$ is the group consisting of the four elements $\pm\mathbf{a}$ and ± 1. Thus, the group $\mathcal{H}_1$ is the group generated by a single reflection. The group $2\mathcal{H}_1$ consists of the two elements ± 1 while the corresponding rotation group $\mathcal{C}_1$ contains only the identity element 1. Either of these last two groups can be regarded as the symmetry group of a figure with no symmetry at all.

A symmetry group with a fixed point is called a *point group*. The groups $\mathcal{H}_p$ and $\mathcal{C}_p$, for any positive integer p, are point groups in two dimensions. The groups $2\mathcal{H}_p$ and $2\mathcal{C}_p$ are oriented point groups. The point groups of a few simple 2-dimensional figures are given in Fig. 3. Besides $\mathcal{H}_p$ and $\mathcal{C}_p$, there are no other point groups in two dimensions. This can be proved by considering the possibility of a group generated by three distinct vectors $\mathbf{a}$, $\mathbf{b}$, $\mathbf{c}$ in the same plane. If they are to be generators of a symmetry group, then each pair of them must be related by a dicyclic condition like (14). It can be proved, then that one of the vectors can be generated from the other two, so two vectors suffice to generate any symmetry group in two dimensions.

Although it takes us outside the domain of finite groups, it is worthwhile to consider the limiting case $p = \infty$. With increasing values of p, a regular p-sided

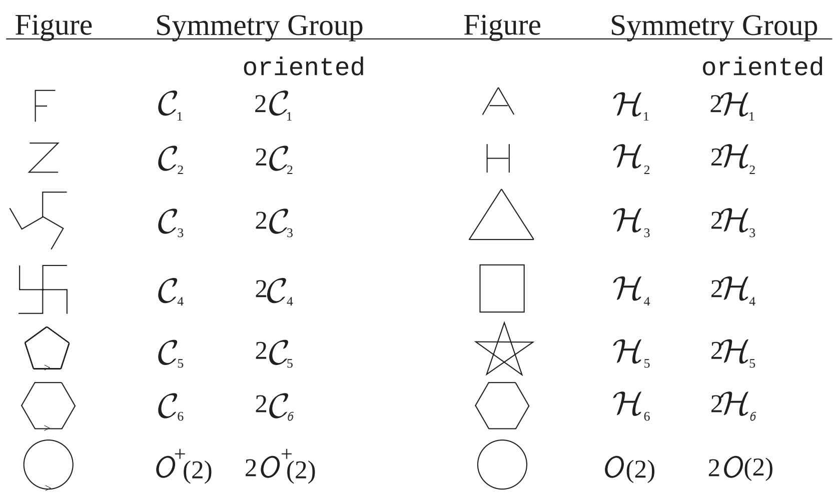


Fig. 3. Symmetry groups of some 2-dimensional figures.

polygon is an increasingly good approximation to a circle, which can be regarded as the limit at $p = \infty$. Therefore, the complete orthogonal group $O(2)$ in two dimensions can be identified as the symmetry group of a circle, the rotation subgroup of $O^+(2)$. It can be regarded as the symmetry group of an oriented circle, as shown in Fig. 3. Note that a reflection will reverse the orientation, so $O(2)$ is the group of an unoriented circle. Note further, by examining Fig. 3, that even for finite p, $\mathcal{C}_p$ is the group of an oriented polygon while $\mathcal{H}_p$ is the group of an unoriented polygon.

Point groups in three dimensions

We have seen how every finite subgroup of the orthogonal group $O(2)$ can be generated by one or two reflections. One might guess, then, that no more than three reflections are required to generate any finite subgroup of the orthogonal group $O(3)$. So we shall see!

If three unit vectors $\mathbf{a}$, $\mathbf{b}$, $\mathbf{c}$ are to be generators of a finite multiplicative group, then each pair of vectors must generate a finite subgroup, so we know from our preceding analysis that they must satisfy the *dicycle conditions*

$$(\mathbf{ab})^p = (\mathbf{bc})^q = (\mathbf{ac})^r = -1\,, \tag{15}$$

where p, q, and r are positive integers. If $r = 1$, then (15) implies $\mathbf{c} = -\mathbf{a}$, and $p = q$, so (15) reduces to a relation between two vectors, the case we have already considered. Therefore, if the vectors $\mathbf{a}$, $\mathbf{b}$, and $\mathbf{c}$ are to be distinct, then each of the integers p, q, and r must be greater than 1.

The three generators of rotations in (15) are not independent, for they are related by the equation

$$(\mathbf{ab})(\mathbf{bc}) = \mathbf{ac}\,. \tag{16}$$

We have seen in Sec. 2-4 that this equation relates the sides of a spherical triangle with vertices $\mathbf{a}$, $\mathbf{b}$, and $\mathbf{c}$. This relation restricts the simultaneous values allowed for $\mathbf{p}$, $\mathbf{q}$, and $\mathbf{r}$ in (15). The precise nature of the restriction can be ascertained by writing (15) in the equivalent form

$$\begin{aligned} \mathbf{ab} &= e^{i\mathbf{c}'\pi/p}, \\ \mathbf{bc} &= e^{i\mathbf{a}'\pi/q}, \\ \mathbf{ac} &= e^{i\mathbf{b}'\pi/r}. \end{aligned} \tag{17}$$

The unit vectors $\mathbf{a}'$, $\mathbf{b}'$, $\mathbf{c}'$ are *poles* (or axes) of the rotations generated by $\mathbf{ab}$, $\mathbf{bc}$, $\mathbf{ac}$, so the spherical triangle they determine is aptly called the*polar triangle* of the generating triangle $\{\mathbf{a}, \mathbf{b}, \mathbf{c}\}$. From (17) it follows that the interior angles of the polar triangle are equal in magnitude to corresponding sides of the generating triangle and they have the values π/p, π/q and π/r. Therefore,

Oriented Point Group Symbol	Generators	Point Group Symbol
$[pq]$	$\mathbf{a},\ \mathbf{b},\ \mathbf{c}$	pq
$[\bar{p}q]$	$\mathbf{ab},\ \mathbf{c}$	$\bar{p}q$
$[p\bar{q}]$	$\mathbf{a},\ \mathbf{bc}$	$p\bar{q}$
$[\bar{p}\bar{q}]$	$\mathbf{ab},\ \mathbf{bc}$	$\bar{p}\bar{q}$
$[\overline{pq}]$	$\mathbf{abc}$	$\overline{pq}$
$[p]$ or $2\mathcal{D}_p$	$\mathbf{a},\ \mathbf{b}$	p or $\mathcal{D}_p$
$[\bar{p}]$ or $2\mathcal{H}_p$	$\mathbf{ab}$	pq or $\mathcal{H}_p$

Table 2 Symbols for the double point (diorthogonal) groups in three dimensions and their corresponding point (orthogonal) groups. The groups generated by three unit vectors have the presentation

$$(\mathbf{ab})^p = (\mathbf{bc})^q = (\mathbf{ac})^2 = -1\,,$$

with $5 \geq p \geq q \geq 2$. The groups generated by two unit vectors have the presentation

$$(\mathbf{ab})^p = -1\,.$$

Of course, our notation admits confusion between $p = 22$ and $pq = 22$, but we will not be concerned with such large values for p.

according to the "spherical excess formula" (established in Ex. 2-4.20), the area Δ' of the polar triangle is given by

$$\Delta' = \pi\Big(\frac{1}{p} + \frac{1}{q} + \frac{1}{r} - 1\Big)\,. \tag{18}$$

This is the desired relation among p, q, and r in its most convenient form.

From (18) we can determine the permissible values of p, q, and r. Since the area Δ' must be positive, equation (18) gives us the inequality

$$\frac{1}{p} + \frac{1}{q} + \frac{1}{r} > 1\,. \tag{19}$$

The integer solutions of this inequality are easily found by trial and error. Trying $p = q = r = 3$, we see that there are no solutions with $p > q > r > 2$. So, without loss of generality, we can take $r = 2$ so (19) reduces to

$$\frac{1}{p} + \frac{1}{q} > \frac{1}{2}\,. \tag{20}$$

Requiring $p \geq q$, we see that any value of p is allowed if $q = 2$, and if $q = 3$, we find that $p = 3$, 4 or 5. This exhausts the possibilities. It is not difficult to prove that no new point groups with four or more generating vectors are possible. For every subset of three vectors must generate one of the groups we have already found, and it follows from this that if we have four generators, then one of them can be generated from the other three.

All we need now is a suitable nomenclature to express our results in a compact form. Since each of the multiplicative groups generated by three unit vectors is distinguished by the values of p, q and $r = 2$ in the presentation (15), each of these finite diorthogonal groups can be identified by the symbol $[pq]$. Let us use the simpler symbol pq for the corresponding orthogonal groups, because they are more prominent in the literature of mathematics and physics. The groups pq are usually called *point groups* by physicists, who usually refer to the groups $[pq]$ as *double point groups*, though considering the geometrical reason for the doubling, it might be better to call them *oriented point groups.* The usual derivation of the double groups is far more complicated than the one presented here. Consequently, the double groups are seldom mentioned except in the most esoteric applications of group theory to physics. Of course, we have seen that there is ample reason to regard the diorthogonal groups as more fundamental than the orthogonal groups. Even so, we have learned that the diorthogonal and orthogonal groups are so simply and intimately related that we hardly need a special notation to distinguish them.

Without altering the group presentation (15), we get subgroups of $[p\,q]$ by taking the various products of the vectors $\mathbf{a}$, $\mathbf{b}$, $\mathbf{c}$ as generators. To denote these groups, let us introduce the notation $\bar{p}$ to indicate a generator $\mathbf{ab}$ satisfying the relation $(\mathbf{ab})^p = -1$. Accordingly, $[\bar{p}\,\bar{q}\,]$ denotes the dirotation group generated

Table 3. The 32 crystal classes (point groups).

	Class				
System	Geometric	Schoen-flies	Inter-national	Order	Number of Space Groups
Triclinic	1	$\mathcal{C}_1$	1	1	1
	$\overline{22}$	$\mathcal{S}_2 = \mathcal{C}_i$	$\bar{1}$	2	1
Monoclinic	$\bar{2}$	$\mathcal{C}_2$	2	2	3
	1	$\mathcal{C}_{1h} = \mathcal{C}_s$	m	2	4
	$2\bar{2} = \bar{2}2$	$\mathcal{C}_{2h}$	2/m	4	6
Orthorhombic	$\bar{2}\bar{2}$	$\mathcal{D}_2 = \mathcal{V}$	222	4	9
	2	$\mathcal{C}_{1v}$	mm2	4	22
	22	$\mathcal{D}_{2h} = \mathcal{V}_h$	mmm	8	28
Tetragonal	$\bar{4}$	$\mathcal{C}_4$	4	4	6
	$\overline{42}$	$\mathcal{C}_4$	$\bar{4}$	4	2
	$\bar{4}2$	$\mathcal{C}_{1h}$	4/m	8	6
	$\bar{4}\bar{2}$	$\mathcal{D}_4$	422	8	10
	4	$\mathcal{C}_{4v}$	4mm	8	12
	$4\bar{2}$	$\mathcal{D}_{2d} = \mathcal{V}_d$	$\bar{4}2$m	8	12
	42	$\mathcal{D}_{2h}$	4/mmm	16	20
Trigonal (Rhombohedral)	$\bar{3}$	$\mathcal{C}_3$	3	3	4
	$\overline{62}$	$\mathcal{S}_6 = \mathcal{C}_{3i}$	$\bar{3}$	6	2
	$\bar{3}\bar{2}$	$\mathcal{D}_3$	32	6	7
	3	$\mathcal{C}_{3v}$	3m	6	6
	$6\bar{2}$	$\mathcal{D}_{3d}$	$\bar{3}$m	12	6
Hexagonal	$\bar{6}$	$\mathcal{C}_3$	6	6	6
	$\bar{3}2$	$\mathcal{C}_{3h}$	$\bar{6}$	6	1
	$\bar{6}2$	$\mathcal{C}_{6h}$	6/m	12	2
	$\bar{6}\bar{2}$	$\mathcal{D}_6$	622	12	6
	6	$\mathcal{C}_{6v}$	6mm	12	4
	32	$\mathcal{D}_{3h}$	$\bar{6}$m2	12	4
	62	$\mathcal{D}_{6h}$	6/mmm	24	4
Cubic	$\bar{3}\bar{3}$	$\mathcal{T}$	23	12	5
	$4\bar{3}$	$\mathcal{T}_h$	m3	24	7
	$\bar{4}\bar{3}$	$\mathcal{O}$	432	24	8
	$33 = \bar{3}3$	$\mathcal{T}_h$	$\bar{4}$3m	24	6
	$43 = \bar{4}3$	$\mathcal{O}_h$	m3m	48	10
					230

by $\mathbf{ab}$ and $\mathbf{bc}$, and $\bar{p}\,\bar{q}$ denotes the corresponding rotation group. The notation is explained further and the various groups it denotes are listed in Table 2.

Now that we have a compact notation, we list in Table 3 all the point groups in three dimension, that is, all the finite subgroups of $O(3)$. We begin by listing the groups pq for the allowed values of p and q determined above. Then we apply the "overbar notation" to generate a list of candidate subgroups $\bar{p}\,\bar{q}$, $\bar{p}\,q$, $p\bar{q}$, $\overline{pq}$. Finally, we check the candidates to see if they are new symmetry groups.

The groups pq are said to be *finite reflection groups*, because they are generated by reflections. All the finite groups are reflection groups or subgroups thereof. The groups pq generated by two pairs of reflections are *finite rotation groups*. Table 3 shows that the only finite rotation groups are the cyclic groups $\bar{p} = \mathcal{C}_p$, the dihedral groups $\bar{p}\bar{2} = \mathcal{D}_p$, the tetrahedral group $\overline{33} = \mathcal{T}$, the octahedral group $\overline{43} = O$ and the icosahedral group $\overline{53} = \mathcal{I}$. These are the only finite groups with widely accepted names. The last three of them are symmetry groups of the famous Platonic solids, the five regular solids discovered by the ancient Greeks (Fig. 4). The tetrahedral group is the rotational symmetry group of a tetrahedron. The octahedral group $\overline{43}$ is the rotational symmetry group of both the (8-sided) octagon and the (6-sided) cube. The icosahedral group $\overline{53}$ is the symmetry group of both the (20-sided) icosahedron and the (12-sided) dodecahedron. As can be seen by looking at Fig. 4, the notation $\overline{53}$ indicates the fivefold symmetry at each vertex (face) and the threefold symmetry at each face (vertex) of the icosahedron (dodecahedron). The notation $\overline{43}$ and $\overline{33}$ have similar interpretations for the other regular solids. From the fact that there are no other rotational symmetry groups besides those we have mentioned, it is not difficulty to prove that there are no regular convex polyhedra besides the Platonic solids. There exist, however, some regular solids which are "starshaped" and so not convex. The largest symmetry groups of the Platonic solids are actually the reflection groups 33, 43 and 53 rather than their rotational subgroups, but this was not appreciated when names were handed out, so they are without special names.

The cyclic and dihedral groups are symmetry groups for various prisms or prismatic crystals rather than polyhedra. However, in physics they appear most frequently as symmetry groups for molecules. We are now in position to see that the dihedral group $\mathcal{D}_6 = \overline{62}$, rather than the cyclic group $\mathcal{C}_6 = 6$, is the rotational symmetry group for the Benzene molecule (Fig. 1) in a space of three dimensions rather than two. Furthermore, it is readily verified (Ex. 2) that the rotation group $\mathcal{D}_6 = \overline{62}$ is isomorphic to the reflection group $\mathcal{H}_6 = 6$, and they have identical effects on the planar Benzene molecule; nevertheless, they have different geometrical effects on three dimensional objects. In three dimensions the complete symmetry group of the Benzene molecule is the reflection group $\mathcal{D}_{6h} = 62$, which is formed by using the generating vector $\mathbf{c}$ along with the reflection generators $\mathbf{a}$ and $\mathbf{b}$ of $\mathcal{H}_6 = 6$, as illustrated in Fig. 1.

Besides the groups pq generated by reflections and the groups $\bar{p}\,\bar{q}$ generated by rotations, Table 3 lists "mixed groups" $\bar{p}\,q$, $p\bar{q}$ and $\overline{pq}$ generated by com-

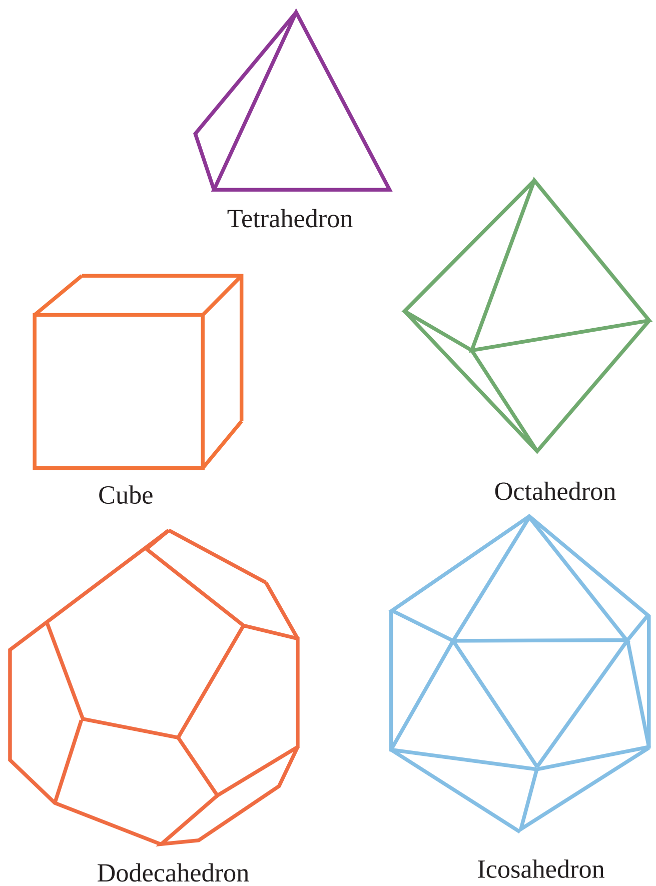


Fig. 4. The five regular (convex) polyhedra. A polyhedron is *regular* is all its faces are identical regular polygons. Note that an octagon can be formed from a cube (or vice versa) by joining the midpoints of adjacent faces with line segments, that is, one can be formed from the other by interchanging vertices and faces. The dodecahedron and the icosahedron are similarly related. What about the tetrahedron?

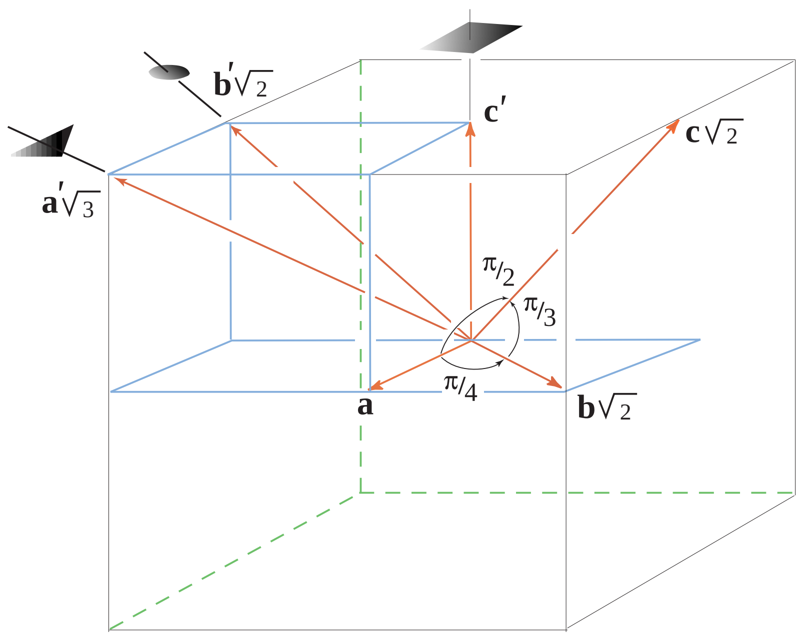


Fig. 5. Generators **a**, **b**, **c** for the double point group [43] of a cube or an octagon. Vertices **a**′, **b**′, **c**′ of the polar triangle (or fundamental region) specify axes of threefold, twofold, and fourfold symmetry, as indicated by the triangle, lense, and square symbols.

binations of rotations and reflections. Some of the mixed groups are identical to reflection groups. For example, the equivalence $43 = \overline{4}3$ means that $\mathbf{a}$, $\mathbf{b}$, $\mathbf{c}$ generate the same group as $\mathbf{ab}$, $\mathbf{c}$; in other words, the group 43 generated by three reflections can also be generated by one rotation and one reflection.

Some of the candidates for mixed groups must be rejected because they do not satisfy the condition for a symmetry group. To see why, consider the rotary-reflection group $\overline{pq}$. The corresponding diorthogonal group $[\overline{pq}]$ has the same generator $\mathbf{abc}$. Since $\mathbf{ab}$ represents a rotation and $\mathbf{c}$ represents a reflection, the product $\mathbf{abc}$ represents a combined rotation and reflection, that is, a rotary-reflection. The quantity $R = (\mathbf{abc})^2$ is an even spinor generating a dirotational subgroup of $[\overline{pq}]$, so it must satisfy the dicyclic condition $R^n = (\mathbf{abc})^{2n}$ (for some integer n) if $[\overline{pq}]$ is to be a symmetry group. This condition must be evaluated separately for each group. For example, for the group $[\overline{p2}]$, the vector $\mathbf{c}$ is orthogonal to both vectors $\mathbf{a}$ and $\mathbf{b}$, hence $\mathbf{abc} = \mathbf{cab}$ and

$$R = (\mathbf{abc})^2 = (\mathbf{ab})^2. \tag{21}$$

But $(\mathbf{ab})^p = -1$, so

$$R^p = (\mathbf{abc})^{2p} = (\mathbf{ab})^{2p}. \tag{22}$$

Therefore, the dicyclic condition $R^n = -1$ can be met only if $p = 2n$, that is, only if p is an even integer. Thus, we have proved that the group $\overline{p2}$ is a symmetry group only if p is even, as stated in Table 3. The same argument proves that $p\overline{2}$ is a symmetry group only for even p. In a similar way, it can be proved that $\overline{33}$, $\overline{43}$ and $\overline{53}$ are not symmetry groups, but the algebra required is a little trickier.

Our "geometric notation" for the finite groups is unconventional, so Table 3 relates it to the widely used Shoenflies notation to facilitate comparison with the literature on crystallography and group theory. The rationale for the Schoenflies notation need not be explained here. However, it should be noted that our geometric notation has the great advantage of enabling us to write down immediately the generators and relations for any finite group by employing the simple code in Table 2. Thus, for the group $[43]$, the angle between generators $\mathbf{a}$ and $\mathbf{b}$ is $\pi/4$, the angle between $\mathbf{b}$ and $\mathbf{c}$ is $\pi/3$, and the angle between $\mathbf{a}$ and $\mathbf{c}$ is $\pi/2$. Figure 5 shows three such vectors in relation to a cube whose reflection group they generate. According to (17), the algebraic relations among the generators are fully expressed by the equations

$$\mathbf{ab} = e^{i\mathbf{c}'\pi/4}, \tag{23}$$

$$\mathbf{bc} = e^{i\mathbf{a}'\pi/3}, \tag{24}$$

$$\mathbf{ac} = e^{i\mathbf{b}'\pi/2} = i\mathbf{b}'\,. \tag{25}$$

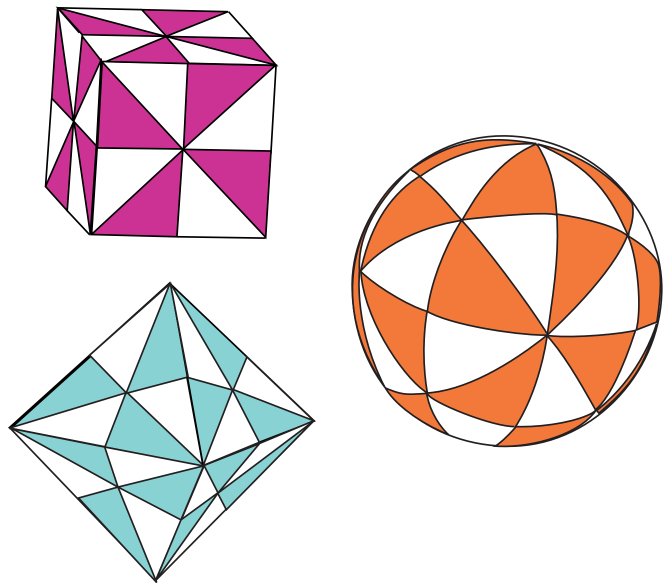


Fig. 6a. Fundamental regions for the reflection group $43 = O$ on the surface of a cube, an octagon, or a sphere.

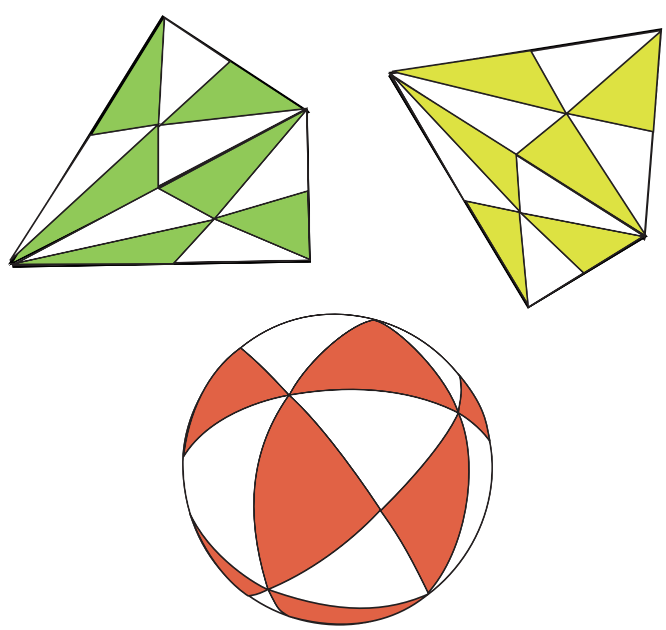


Fig. 6b. Fundamental regions for the group $53 = \tilde{I}_h$.

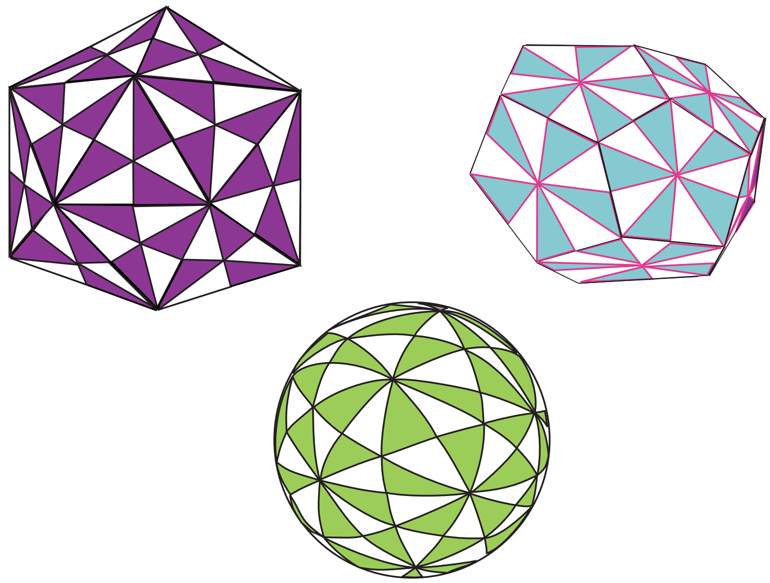


Fig. 6c. Fundamental regions for the group $33 = \tilde{t}_d$.

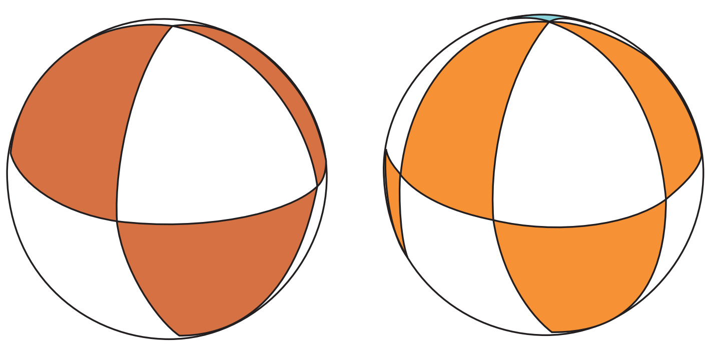


Fig. 6d. Fundamental regions for the groups $22 = \mathcal{D}_2$ and $32 = \mathcal{D}_3$.

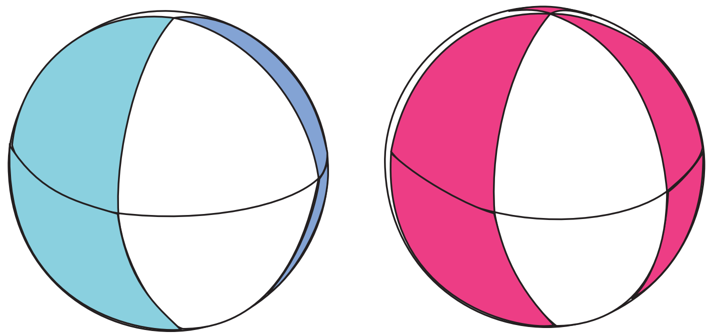


Fig. 6e. Fundamental regions for the group $2 = \mathcal{H}_2$ and $3 = \mathcal{H}_3$.

The poles $\mathbf{a}'$, $\mathbf{b}'$, $\mathbf{c}'$ are also shown in Fig. 5, It should be evident from Fig. 5 that every reflection symmetry of the cube is generated by a vector directed at the center of a face (like $\mathbf{a}$) or at the midpoint of an edge (like $\mathbf{b}$ or $\mathbf{c}$). Furthermore, every one of these vectors is also the pole of a four-fold rotation symmetry (like $\mathbf{c}'$ or $\mathbf{a}$) or of a two-fold rotation symmetry (like $\mathbf{b}'$, $\mathbf{b}$ or $\mathbf{c}$) but not of a three-fold symmetry (like $\mathbf{a}'$). Indeed, we see from Fig. 5 that $\mathbf{b}'$ can be obtained from $\mathbf{c}$ by a rotation generated by $(\mathbf{ab})^2 = e^{i\mathbf{c}'\pi}$ about the $\mathbf{c}'$ axis, so we can directly write down the relation

$$\mathbf{b}' = (\mathbf{ba})^2\mathbf{c}(\mathbf{ab})^2 \,. \tag{26}$$

Similarly, by a rotation about the $\mathbf{a}'$ axis,

$$\mathbf{c}' = (\mathbf{cb})\mathbf{a}(\mathbf{bc}) = \mathbf{cbabc} \,. \tag{27}$$

This illustrates how algebraic relations in the group [43] can be written down directly and interpreted by referring to some model of a cube like Fig. 5. A three-dimensional physical model of a cube is even more helpful than a figure.

The polar triangle with vertices $\mathbf{a}'$, $\mathbf{b}'$, $\mathbf{c}'$ determines a triangle on the surface of a cube, shown as a shaded triangle in Fig. 5. This triangle is called a fundamental region of the group 43 for the following reason. Notice that each of the three generators $\mathbf{a}$, $\mathbf{b}$, $\mathbf{c}$ is perpendicular to one of the three sides of the triangle, so a reflection by any one of the generators will transform the triangle into an adjacent triangle of the same size and shape. By a series of such reflections the original triangle can be brought to a position covering any point on the cube. In other words, the entire surface of the cube can be partitioned into triangular fundamental regions, as shown in Fig. 6a, so that any operation of the group 43 simply permutes the triangles. Fig. 6a shows an alternative partition of the octahedron and the sphere into fundamental regions of the group 43. In a completely analogous way, the tetrahedron and the icosahedron (or dodecahedron) can be partitioned into fundamental regions of the groups 33 and 53 respectively, as shown in Fig. 6b, c. The sphere can also be partitioned into fundamental regions for the groups p2 and p, as illustrated in Fig. 6d, e, though in the latter case the fundamental regions are "lunes" rather than triangles.

Given one fundamental region of a group, there is one and only one group operation which transforms it to any one of the other fundamental regions. Consequently, the order of a group is equal to the number of distinct fundamental regions. Thus, from Fig. 6a we see that there are eight fundamental regions on the face of a cube, so there are $6 \times 8 = 48$ elements in the group 43. To get a general formula for the order of finite groups, it is better to consider fundamental regions on a unit sphere. Then the area of each fundamental region is equal to the area of the polar triangle given by (18), so the order of the group is obtained by dividing this into the area 4π of the sphere. For example, taking $r = 2$ and $q = 3$ in (18), we find that the orders of the reflection groups $p3$ are given by

$$\frac{4\pi}{\delta'} = \frac{2p}{6-p}\,. \tag{28}$$

This is twice the order of the rotation groups $\bar{p}\bar{3}$, because all rotations are generated by pairs of reflections. The orders of the other finite groups and their subgroups can be found in a similar way. The results are listed in Table 3.

The 32 Crystal Classes and 7 Crystal Systems

A *crystal* is a system of identical atoms or molecules located near the points of a lattice. A 3-dimensional *lattice* is a descrete set of points generated by three linearly independent vectors $\mathbf{a}_1$, $\mathbf{a}_2$, $\mathbf{a}_3$. Any $\mathbf{t}_n$ in the lattice can be expressed as a linear combination of the generators with integer coefficients, that is,

$$\mathbf{t}_n = n_1\mathbf{a}_1 + n_2\mathbf{a}_2 + n_3\mathbf{a}_3\,, \tag{29}$$

where n_1, n_2, n_3 are integers. Given the generating vectors, any set of integers $n = \{n_1, n_2, n_3\}$ determines a lattice point, so the lattice is an infinite set of points. Of course, any crystal consists of only a finite number of atoms, but the number is so large that for the analysis of many crystal properties it can be regarded as infinite without significant error. Our aim here is to classify crystals according to the symmetries they possess. The symmetries of a crystal depend only on the locations of its atoms and not on the physical nature of the atoms. Therefore, the analysis of crystal symmetries reduces to the analysis of lattice symmetries, a well-defined geometrical problem.

Like any finite object, the symmetry of a lattice is described by its symmetry group, the complete group of isometries that leave it invariant. However, unlike the group of a finite object, the symmetry group of a lattice includes translations as well as orthogonal transformations. Before considering translations, let us determine the conditions for a lattice to be invariant under one of the point groups.

Lattice calculations are greatly facilitated by introducing the reciprocal frame $\{\mathbf{a}_k^*\}$. Reciprocal frames were introduced (with a different notation) and their properties were analyzed in Ex. (2-3.11). Presently, all we need are the relations

$$\mathbf{a}_j^* \cdot \mathbf{a}_k = \delta_{jk} \,, \tag{30}$$

for $j, k = 1,\ 2,\ 3$, which determine the reciprocal frame uniquely.

Now, any symmetry $\mathcal{S}$ of a lattice transforms lattice points $\mathbf{a}_k$ $(k = 1, 2, 3)$ into new lattice points

$$\mathbf{s}_k = \mathcal{S}\mathbf{a}_k = \sum_j a_j \, s_{jk} \,, \tag{31}$$

where the matrix elements

$$s_{jk} = \mathbf{a}_j^* \cdot \mathbf{s}_k = \mathbf{a}_j^* \cdot (\mathcal{S}\mathbf{a}_k) \tag{32}$$

are all integers. Consequently, the trace of this matrix

$$\sum_k s_{kk} = \sum_k \mathbf{a}_k^* \cdot (\mathcal{S}\mathbf{a}_k) \tag{33}$$

is also an integer. This puts a significant restriction on the possible symmetries of a lattice. In particular, if $\mathcal{R}$ is a rotation symmetry generating a rotation subgroup, then it satisfies a cyclic condition $\mathcal{R}^p = 1$, and it rotates the lattice through an angle $\theta = 2\pi/p$. From Ex. (3.12), we know that

$$\operatorname{Tr} \mathcal{R} = \sum_k \mathbf{a}_k^* \cdot (\mathcal{R}\mathbf{a}_k) = 1 + 2\cos\theta \,. \tag{34}$$

This has integer values only if

$$\cos\theta = 0,\ \pm\tfrac{1}{2},\ \pm 1 \,, \tag{35}$$

which has the solutions

$$\theta = 0,\ \frac{\pi}{3},\ \frac{\pi}{2},\ \frac{2\pi}{3},\ \pi,\ \frac{4\pi}{3},\ \frac{3\pi}{2},\ \frac{5\pi}{3},\ 2\pi \,. \tag{36}$$

Consequently, the order p of any cyclic subgroup of a lattice point group is restricted to the values

$$p = 1,\ 2,\ 3,\ 4,\ 6 \,. \tag{37}$$

This is known as the *crystallographic restriction.*

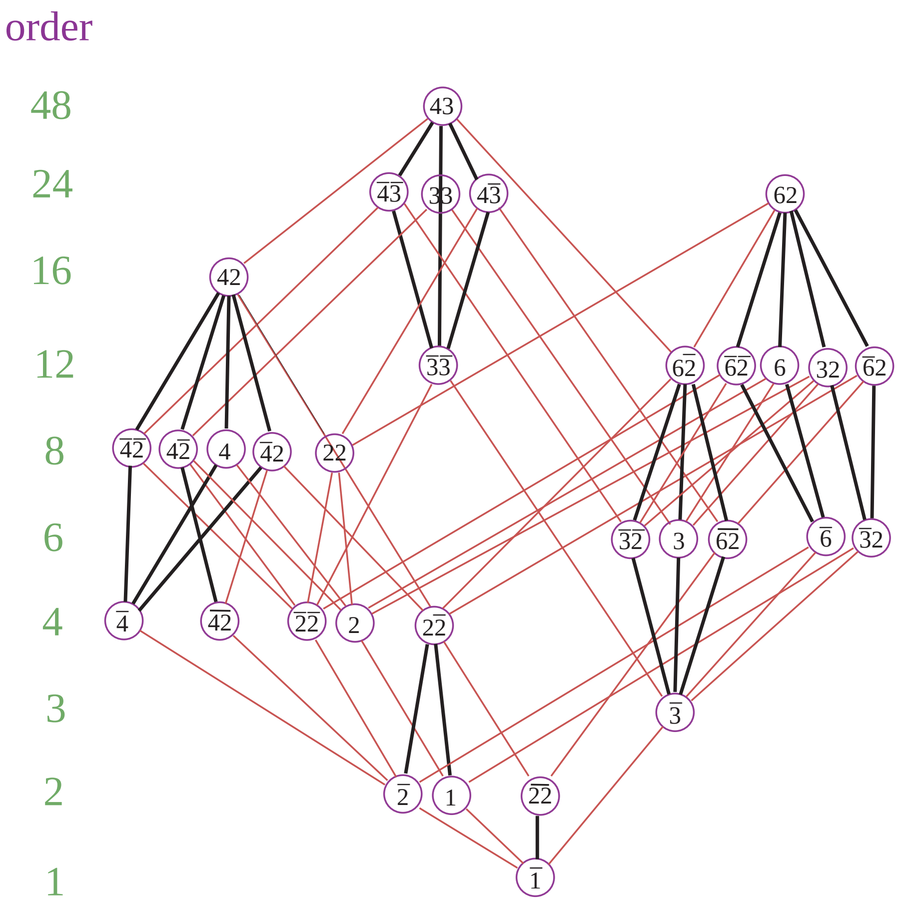


Fig. 7. Subgroup relations among the 32 crystallagraphic point groups. Dark lines connect groups in the same crystal system.

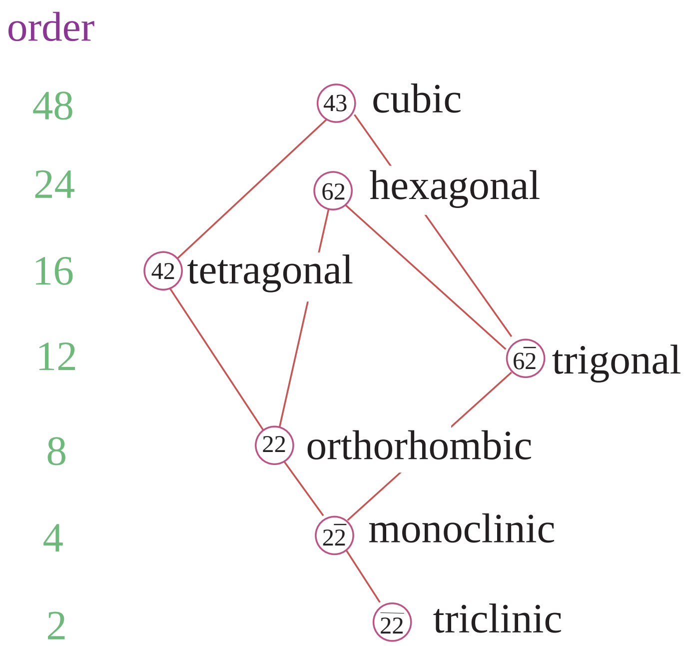


Fig. 8. Subgroup relations for the seven holohedry.

The point groups satisfying crystallographic restriction are called *crystallographic point groups*. There are exactly 32 of them. They are listed in Table 4. Crystals are accordingly classified into 32 *crystal classes*, each one corresponding to one of the point groups. Besides our geometric symbols for the crystal classes (point groups) and the symbols of Schoenflies, Table 4 lists symbols adopted in the *International Tables of X-Ray Crystallography*, an extensive standard reference on the crystallographic groups.

It is conventional to subdivide the crystal classes into *seven crystal systems* with the names given in Table 4. This subdivision corresponds to an arrangement of the point groups into families of subgroups, as indicated in Fig. 7. The largest group in each system is called the *holohedry* of the system. Relations of one system to another are described by the subgroup relations among their holohedry, as shown in Fig. 8. From the symbols, it is easy to produce a set of generators for each of the seven diholohedry (the spinor groups of the holohedry). Figure 9 has sets of such generators arranged to show the simple relations among them. Note that the orthogonal vectors $\mathbf{a}$, $\mathbf{c}$ can be chosen to be the same for each system, and there are three distinct choices for the remaining vector $\mathbf{b}$. Actually, from the generators for $[43|$ and $[62]$ the generators of all other crystallographic point groups can be generated, because all the groups are subgroups of $[43]$ or $[62]$, as shown in Fig. 7.

We have determined all possible point symmetry groups for 3-dimensional objects. There are, however, an infinite number of different objects with the same symmetry group, for a symmetry group describes a relation among identical parts of an object without saying anything about the nature of those parts. Figure 10 shows a set of objects with symmetries of the 32 crystallographic point groups.

The Space Groups

A set of linearly independent vectors $\mathbf{a}_1$, $\mathbf{a}_2$, $\mathbf{a}_3$ (and their negatives $-\mathbf{a}_1$, $-\mathbf{a}_2$, $-\mathbf{a}_3$) generate a discrete group under addition, and each element can be associated with a lattice point designated by (29). We call this the *translation group* of the lattice. It is an additive symmetry group of the corresponding lattice. We have seen also that there are 32 point groups that may leave a lattice invariant. The complete symmetry group of a crystal is called its *space group*. Each element of a space group can be written as an orthogonal transformation combined with a translation, as represented by (1). Consequently, every space group can be described as a point group combined with a translation group, and we can determine all possible space groups by finding all possible combinations. An enumeration of the space groups is of great interest because it characterizes the structure of any regular crystal that might be found in nature. Our purpose now is to see how this can be done.

The translation group of a crystal is an *additive group* generated by three vectors $\mathbf{a}_1$, $\mathbf{a}_2$, $\mathbf{a}_3$, while the double point group is a *multiplicative group* gen-

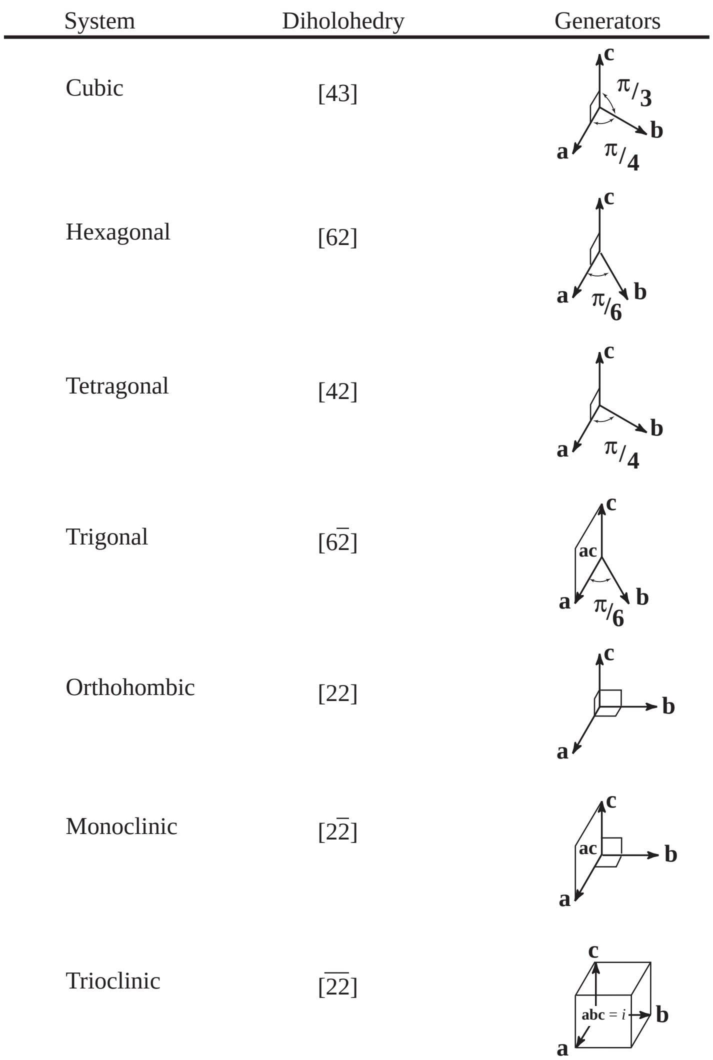


Fig. 9. Generators for the seven diholohedry. One of the generators of $[2\bar{2}]$ and $[6\bar{2}]$ is a bivector **ac**, and the generator of $[\overline{22}]$ is the unit trivector $\mathbf{abc} = i$. All other generators are vectors.

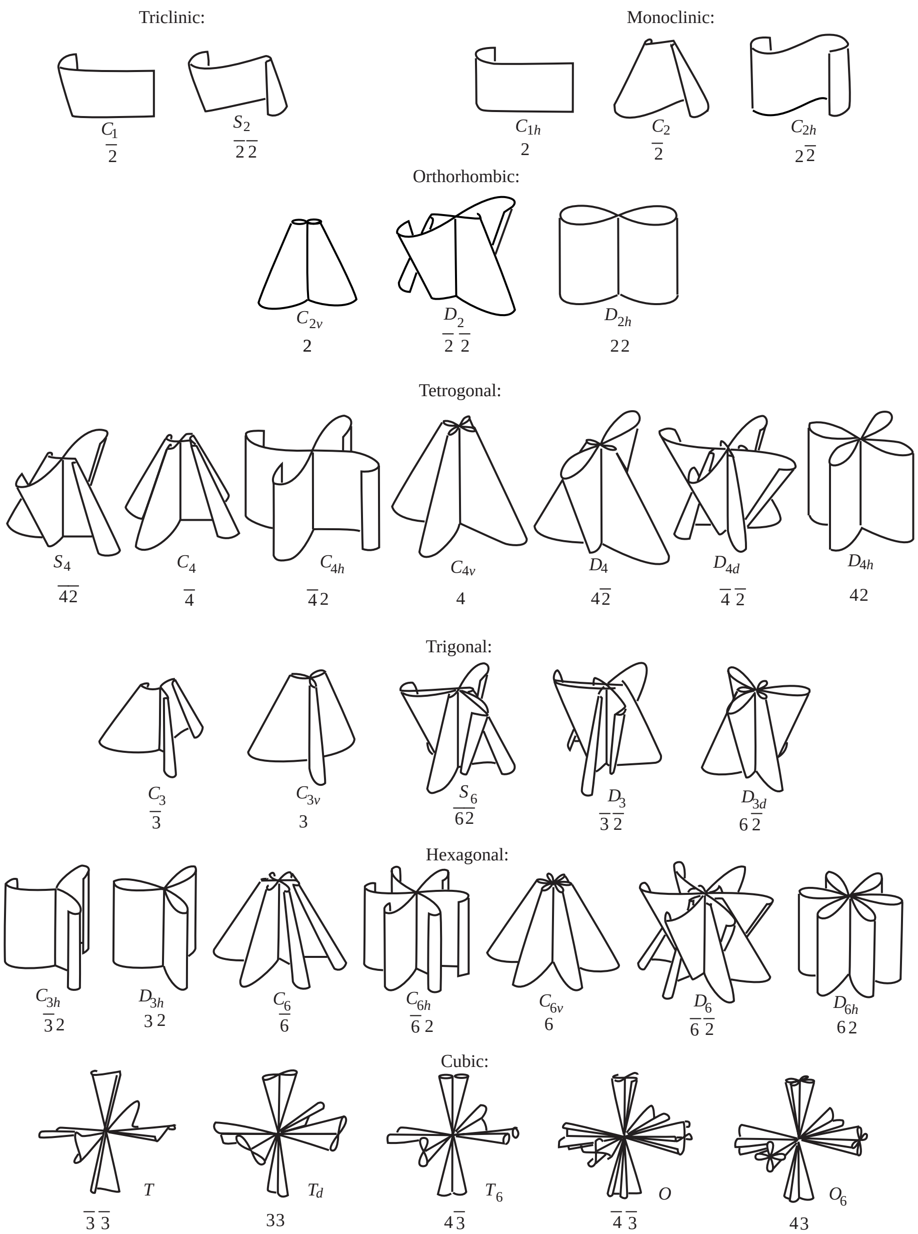

Triclinic:
Monoclinic:
Orthorhombic:
Tetrogonal:
Trigonal:
Hexagonal:
Cubic:
C_1 $\bar{2}$
S_2 $\bar{2}\,\bar{2}$
C_{1h} 2
C_2 $\bar{2}$
C_{2h} $2\bar{2}$
C_{2v} 2
D_2 $\bar{2}\,\bar{2}$
D_{2h} 22
S_4 $\overline{42}$
C_4 $\bar{4}$
C_{4h} $\bar{4}2$
C_{4v} 4
D_4 $4\bar{2}$
D_{4d} $\bar{4}\,\bar{2}$
D_{4h} 42
C_3 $\bar{3}$
C_{3v} 3
S_6 $\overline{6}2$
D_3 $\bar{3}\,\bar{2}$
D_{3d} $6\,\bar{2}$
C_{3h} $\bar{3}2$
D_{3h} $3\,2$
C_6 $\bar{6}$
C_{6h} $\bar{6}\,2$
C_{6v} 6
D_6 $\bar{6}\,\bar{2}$
D_{6h} $6\,2$
T $\bar{3}\,\bar{3}$
T_d 33
T_6 $4\bar{3}$
O $\bar{4}\,\bar{3}$
O_6 43

Fig. 10.

erated by at most three vectors **a**, **b**, **c**. Consequently, the space group can be characterized by a set of relations among these two sets of generators. Indeed, we can choose three linearly independent vectors from the two sets and write the others in terms of them. Thus, every element of a space group can be expressed in terms of three vectors which generate translations by addition and orthogonal transformations by multiplication.

Let the three generating vectors of a space group be **a**, **b**, **c**. The allowed lengths and directions of these vectors are limited by the requirement that they generate translations and that each one is the shortest translation vector with its direction. The allowed directions are further limited by requiring that all orthogonal transformations in the space group are generated by products of the vectors. To express the dependence of an isometry on the generating vectors in simple terms, it is convenient to extend our notation for (1) so that

$$\{\lambda R|\mathbf{t}\} = \{R|\mathbf{t}\}\,, \tag{38}$$

where λ is any nonzero scalar. Then, for example, we can write

$$\{\mathbf{a}|\tfrac{1}{2}\mathbf{a}\}\mathbf{x} = -\mathbf{a}^{-1}\mathbf{x}\mathbf{a} + \tfrac{1}{2}\mathbf{a} = -\hat{\mathbf{a}}\mathbf{x}\hat{\mathbf{a}} + \tfrac{1}{2}\mathbf{a} = -\hat{\mathbf{a}}(\mathbf{x} - \tfrac{1}{2}\mathbf{a})\hat{\mathbf{a}}\,. \tag{39}$$

The transformation $\{\mathbf{a}|\frac{1}{2}\mathbf{a}\} = \{\hat{\mathbf{a}}|\frac{1}{2}\mathbf{a}\}$ is an isometry composed of a reflection and a translation, and it can be interpreted as a reflection in a plane with normal $\hat{\mathbf{a}}$ passing through the point $\frac{1}{2}\mathbf{a}$. Since $\{1|\mathbf{a}\}$ is assumed to be the shortest translation with direction $\hat{\mathbf{a}}$, the translation $\{1|\frac{1}{2}\mathbf{a}\}$ cannot belong to the group. Nevertheless, the combined reflection-translation $\{\mathbf{a}|\frac{1}{2}\mathbf{a}\}$ is an element of some space groups, as we shall see.

We can determine all the space groups by taking each of the 32 point groups in turn and considering the various ways it can be combined with translations to produce a space group. Thus, the space groups fall into 32 classes determined by the point groups. The number of space groups in each class is given in Table 4. There are 230 in all. This is too many to consider here, so let us turn to the simpler problem of determining the space groups in two dimensions.

In two dimensions there are 17 space groups falling into 10 crystal classes. Generators for each group are given in Table 5 along with a "Geometric symbol" designed to describe the set of generators in a way to be explained. For reference purposes, the table gives the "short symbols" for space groups adopted in the *International Tables for X-ray Crystallography.* Finally, the table shows that the space groups fall into 5 crystal systems distinguished by the angle between generating vectors. Five lattice related to the 5 systems are shown in Fig. 11.

To see how every 2-dimensional space group can be described in terms of two vectors, let us examine a representative sample of the groups in Table 5. The reader is advised to refer continually to the table while the groups are discussed. In the geometric symbol for each group, the class is indicated by the class (point group) symbol devised earlier, and the translation generators are indicated by letters a and b.

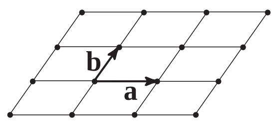
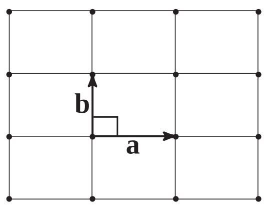
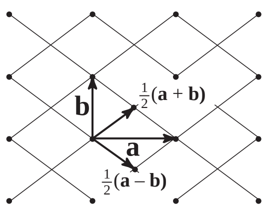
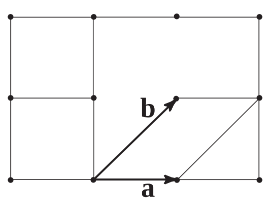
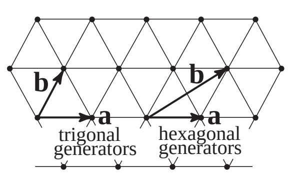
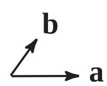
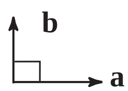
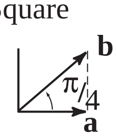
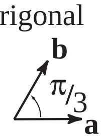
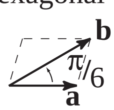
Lattice and Generating Vectors	System and Lattice Type	Lattice Group
	Oblique	$\bar{2}$ ab
	Rectangular	2 ab
	(Centered or Rhombic)	2 $\overline{\text{ab}}$
	Square	4 a
	Hexagonal (Trigonal)	6 a

Fig. 11. The five kinds of planar lattices.

Table 5. The 17 planar space groups.

System	Space Group Symbol: Geometric	Space Group Symbol: International	Space Group Generators
Oblique	$\overline{1}$ ab	p1	$\{1\|\pm\mathbf{a}\}$, $\{1\|\pm\mathbf{b}\}$
	$\overline{2}$ ab	p2	$\{1\|\mathbf{a}\}$, $\{1\|\mathbf{b}\}$, $\{\mathbf{a}\wedge\mathbf{b}\,\|\,\mathbf{0}\}$
Rectangular	1 ab	pm	$\{1\|\pm\mathbf{a}\}$, $\{1\|\pm\mathbf{b}\}$
	1 abg	pg	$\{1\|\mathbf{a}\}$, $\{1\|\pm\mathbf{b}\}$, $\{\mathbf{a}\,\|\,\tfrac{1}{2}\mathbf{b}\}$
	1 $\overline{\text{ab}}$	cm	$\{1\|\tfrac{1}{2}(\mathbf{a}\pm\mathbf{b})\}$, $\{\mathbf{a}\,\|\,\mathbf{0}\}$
	2 ab	pmm	$\{1\|\mathbf{a}\}$, $\{1\|\mathbf{b}\}$, $\{\mathbf{a}\,\|\,\mathbf{0}\}$, $\{\mathbf{b}\,\|\,\mathbf{0}\}$
	2 abg	pmg	$\{1\|\mathbf{a}\}$, $\{1\|\mathbf{b}\}$, $\{\mathbf{a}\,\|\,\tfrac{1}{2}\mathbf{b}\}$, $\{\mathbf{b}\,\|\,\mathbf{0}\}$
	2 abgg	pgg	$\{1\|\mathbf{a}\}$, $\{1\|\mathbf{b}\}$, $\{\mathbf{a}\,\|\,\tfrac{1}{2}\mathbf{b}\}$, $\{\mathbf{b}\,\|\,\tfrac{1}{2}\mathbf{a}\}$
	2 $\overline{\text{ab}}$	cmm	$\{1\|\tfrac{1}{2}(\mathbf{a}+\mathbf{b})\}$, $\{\mathbf{a}\,\|\,\mathbf{0}\}$, $\{\mathbf{b}\,\|\,\mathbf{0}\}$
Square	$\overline{4}$ a	p4	$\{1\|\mathbf{a}\}$, $\{\mathbf{ab}\,\|\,\mathbf{0}\}$
	4 a	p4m	$\{1\|\mathbf{a}\}$, $\{\mathbf{a}\,\|\,\mathbf{0}\}$, $\{\mathbf{b}\,\|\,\mathbf{0}\}$
	4 ag	p4g	$\{1\|\mathbf{a}\}$, $\{\mathbf{a}\,\|\,\tfrac{1}{2}\mathbf{a}\}$, $\{\mathbf{b}\,\|\,\mathbf{0}\}$
Trigonal	$\overline{3}$ a	p3	$\{1\|\mathbf{a}\}$, $\{\mathbf{ab}\,\|\,\mathbf{0}\}$
	3 a	p3m1	$\{1\|\mathbf{a}\}$, $\{\mathbf{a}\,\|\,\mathbf{0}\}$, $\{\mathbf{b}\,\|\,\mathbf{0}\}$
	3 $\overline{\text{ab}}$	p31m	$\{1\|\tfrac{1}{2}(\mathbf{a}+\mathbf{b})\}$, $\{\mathbf{a}\,\|\,\mathbf{0}\}$
Hexagonal	$\overline{6}$ a	p6	$\{1\|\mathbf{a}\}$, $\{\mathbf{ab}\,\|\,\mathbf{0}\}$
	6 a	p6m	$\{1\|\mathbf{a}\}$, $\{\mathbf{a}\,\|\,\mathbf{0}\}$, $\{\mathbf{b}\,\|\,\mathbf{0}\}$

(1) In the group $\overline{1}ab$, the vectors **a** and **b** generate translations only. Since the point group $\overline{1}$ contains only the identity operator, it does not imply any relation between the directions of the translation vectors, so the lattice they generate (Fig. 11) is said to be *Oblique*. The equation

$$\{1|n_1\mathbf{a} + n_2\mathbf{b}\} = \{1|n_1\mathbf{a}\}^{n_1}\{1|n_1\mathbf{b}\}^{n_2} \tag{40}$$

for integers n_1 and n_2 expresses an arbitrary element of the group in terms of the generators.

(2) As indicated in the symbol $\overline{2}$, the group $\overline{2}ab$ contains the 2-fold rotation $\{\mathbf{a}\wedge\mathbf{b}|\mathbf{0}\} = \{\mathbf{i}|\mathbf{0}\}$ determined by the unit bivector **i** for the $\mathbf{a}\wedge\mathbf{b}$-plane. Since

$$\{\mathbf{i}|\mathbf{0}\}\{\mathbf{1}|\mathbf{a}\}\{\mathbf{i}|\mathbf{0}\} = \{\mathbf{1}|-\mathbf{a}\}\,, \tag{41}$$

the negatives of **a** and **b** need not be listed among the translation generators.

The symbol 1 indicates that the groups $1ab$ and $1\overline{ab}$ contain the reflection $\{a|\mathbf{0}\}$. Now $\{a|\mathbf{0}\}$ is required to leave the lattice invariant, so it must transform translation generators into translation generators. By considering the alternatives, one can see that this can be done in two ways only. In the group $1ab$, the reflection is along the direction of one of the translations, so the translation can be reversed by

$$\{\mathbf{a}|\mathbf{0}\}\{\mathbf{1}|\mathbf{a}\}\{\mathbf{a}|\mathbf{0}\} = \{\mathbf{1}|-\mathbf{a}\}\,. \tag{42}$$

The other translation vector **b** must be orthogonal to **a** so that

$$\{\mathbf{a}|\mathbf{0}\}\{\mathbf{1}|\mathbf{b}\}\{\mathbf{a}|\mathbf{0}\} = \{\mathbf{1}|\mathbf{b}\}\,. \tag{43}$$

Since **a** and **b** determine a rectangle, the lattice they generate is said to be *Rectangular*.

The overbar in the symbol $\overline{1}ab$ means that the translation group is generated by $\frac{1}{2}(\mathbf{a}\pm\mathbf{b})$ rather than **a** and **b**. The equation

$$\{\mathbf{a}|\mathbf{0}\}\tfrac{\mathbf{1}}{\mathbf{2}}(\mathbf{a}\pm\mathbf{b}) = -\tfrac{\mathbf{1}}{\mathbf{2}}(\mathbf{a}\pm\mathbf{b})\,. \tag{44}$$

shows that the set of translation generators is invariant under the reflection $\{\mathbf{a}|\mathbf{0}\}$. Since the vectors $\frac{1}{2}(\mathbf{a}\pm\mathbf{b})$ determine a rhombus, the lattice they generate is said to be Rhombic. As Fig. 11 shows, the rhombic lattice can be obtained from the rectangular lattice by inserting a lattice point at the center of each rectangle. For this reason it is sometimes called a *Centered* rectangular lattice.

In the group $1abg$, the reflection indicated by 1 has a relation of the translations different from the one in $1ab$ or $1\overline{ab}$. The symbol g means that the reflection is combined with a translation into a so-called *glide reflection* $\{\mathbf{a}|\frac{1}{2}\mathbf{b}\}$ with $\mathbf{a}\cdot\mathbf{b} = 0$. Neither the reflection $\{\mathbf{a}|\mathbf{0}\}$ nor the translation $\{1|\frac{1}{2}\mathbf{b}\}$ belongs to the symmetry group $1abg$. Consequently, the point group 1 is not a subgroup of $1abg$, as it is for $1ab$ or $1\overline{ab}$. For this reason, the symbol 1 is said to specify the *class* rather than the point group of the spaces groups $1ab$, $1\overline{ab}$ and $1abg$.

It should be easy now to interpret the symbols for the other space groups in Table 5. But a few more comments may be worthwhile. The space groups in the Rectangular and Oblique systems contain two arbitrary parameters, the so-called "lattice constants" $a = |\,\mathbf{a}\,|$ and $b = |\,\mathbf{b}\,|$ which specify the magnitude of the generating translations. This is indicated by the appearance of a and b in the group symbols. On the other hand, a group like $4a$ has only one lattice constant corresponding to a single generating translation. From this one translation all other translations are obtained by operations of the point group.

For the group $4ag$, Table 5 lists $\{\mathbf{a}|\frac{1}{2}\mathbf{a}\}$ instead of a glide-reflection as a generator. The group contains the glide-reflection

$$\{\mathbf{b}|\mathbf{0}\}\{\mathbf{a}|\tfrac{\mathbf{1}}{\mathbf{2}}\mathbf{a}\}\{\mathbf{b}|\mathbf{0}\} = \{\mathbf{a}| - \tfrac{\mathbf{1}}{\mathbf{2}}\mathbf{aba}\}\,, \tag{45}$$

but $\{\mathbf{a}|\frac{1}{2}\mathbf{a}\}$ is preferred as a generator because it is a simpler function of the generating vectors. Like $2abgg$, the group $4ag$ contains two perpendicular glide reflections, but only one of these is counted among the generators, because the other can be obtained from it by a rotation.

It is important to distinguish between a *crystal* or a *pattern* and its lattice. The crystal is a system of similar atoms and a pattern is a system of similar figures located at the-points of a lattice. The space group is a symmetry group of the crystal or pattern, while the lattice has its own symmetry group called a *lattice group.* Although there are 17 different space groups in two dimensions, there are only 5 different lattice groups for the 5 lattice types illustrated in Fig. 11. It will be noted that two distinct lattice types, the Rectangular and the Rhombic, are derived from the same *system* of generating vectors. On the other hand, two distinct generator systems, the Hexagonal and the Trigonal, determine the same lattice.

Patterns with symmetries of each of the 17 planar space groups are shown in Fig. 12 and in Fig. 13.

In three dimensions rotations combine with translation to form screw-displacements, as we have seen in Sec. 5-4. Aside from this, determination of the 230 3-dimensional space groups from the 32 crystal classes involves only consideration like those required to determine the 17 2-dimensional space groups.

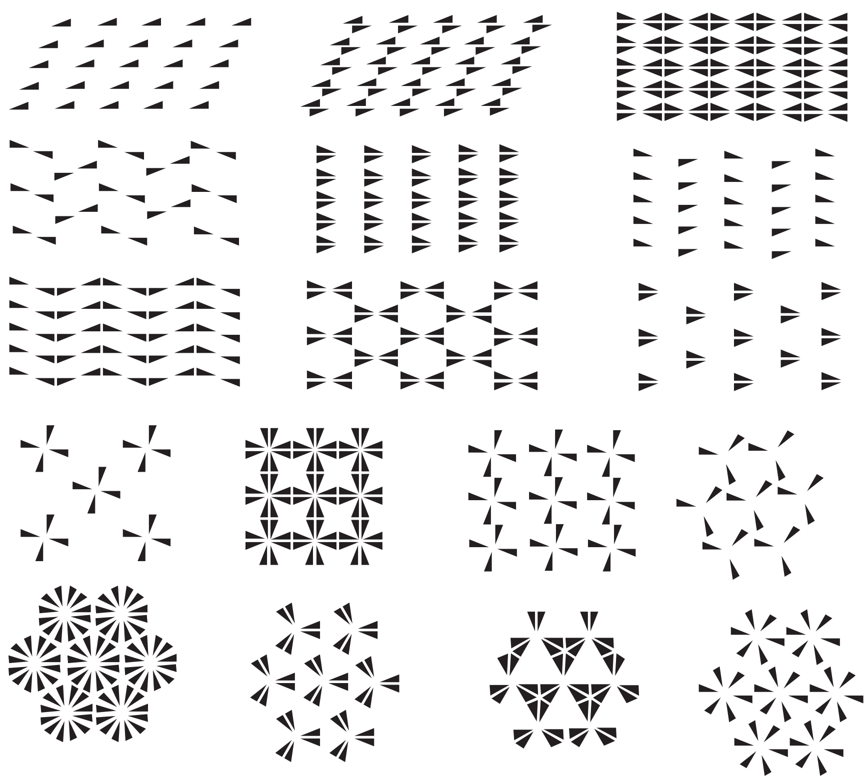


Fig. 12. Regular systems of asymmetrical figures (triangles) corresponding to the 17 symmetry classes of plane patterns (Buerger).

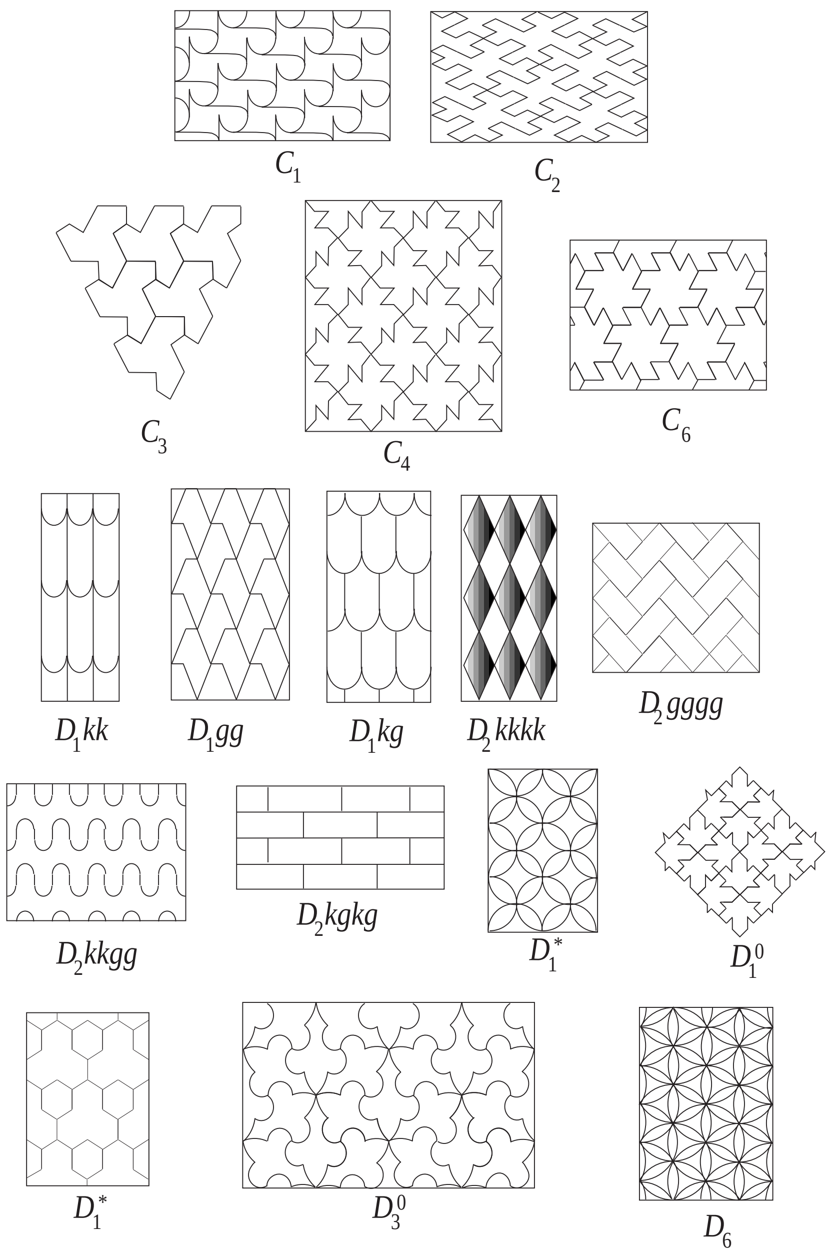


Figure 13. Reprinted with permission from Zeitschrift für Kristallographic.

Exercises

(1) Draw a labeled figure similar to Fig. 2 showing each of the 12 vectors in Table 1.

(2) Prove that the reflection group $\mathcal{H}_p$ is isomorphic to the rotation group $\mathcal{D}_p$

(3) Note that Table 2 does not specify any groups generated by $\mathbf{ac}$ and $\mathbf{b}$. Show that nothing has been lost thereby by identifying the groups in Table 3 generated by $\mathbf{ac}$ and $\mathbf{b}$ for each of the allowed values of p and q.

(4) What group is generated by

$$A = \frac{1}{\sqrt{2}}(1 + i\boldsymbol{\sigma}_1)$$

$$B = \frac{1}{2} + \frac{1}{2}i(\boldsymbol{\sigma}_1 + \boldsymbol{\sigma}_2 + \boldsymbol{\sigma}_3)$$

where $\{\boldsymbol{\sigma}_k\}$ is a standard frame? Determine a complete set of relations for the group by explicit calculation. List all the elements in the group.

(5) Determine relations for the group generated by

$$U = \tfrac{1}{2}(\tau + \boldsymbol{\sigma}_1\boldsymbol{\sigma}_2 + \tau^{-1}\boldsymbol{\sigma}_2\boldsymbol{\sigma}_3)$$

$$V = \tfrac{1}{2}(\tau\boldsymbol{\sigma}_1\boldsymbol{\sigma}_2 + \boldsymbol{\sigma}_2\boldsymbol{\sigma}_3 + \tau^{-1}\boldsymbol{\sigma}_3\boldsymbol{\sigma}_1)$$

where $\tau = \frac{1}{2}(1 + \sqrt{5})$ (the golden ratio!).

(6) From the generators $\mathbf{a}$, $\mathbf{b}$, $\mathbf{c}$ of [43], generate a set of generators for the subgroup [33] and locate them on Fig. 5.

(7) Show that Eq. (18) gives the area of a fundamental region for the group $p = \mathcal{H}_p$, even though that region is not a spherical triangle. Deduce therefrom the order of the group.

(8) How should Eq. (33) be interpreted for negative and zero values of n_1 and n_2? Express $\{1|n_1\mathbf{a} + n_2\mathbf{b}\}^{-1}$ in terms of the generators.

(9) Determine the lattice and generating vectors for each of the patterns in Fig. 12 and 13.

Hints and Solutions

(4) $A^4 = B^3 = (AB)^2 = -1\,;$

$$\pm 2^{-\frac{1}{2}}(1 \pm i\boldsymbol{\sigma}_1)\,, \quad \pm 2^{-\frac{1}{2}}(1 \pm \boldsymbol{\sigma}_2)\,, \quad \pm 2^{-\frac{1}{2}}(1 \pm \boldsymbol{\sigma}_3)$$

$$\tfrac{1}{2} + \tfrac{1}{2}i(\boldsymbol{\sigma}_1 \pm \boldsymbol{\sigma}_2 \pm \boldsymbol{\sigma}_3)$$

$$\pm 2^{-\frac{1}{2}}i(\pm\boldsymbol{\sigma}_1 \pm \boldsymbol{\sigma}_2)\,, \quad \pm 2^{-\frac{1}{2}}i(\pm\boldsymbol{\sigma}_2 \pm \boldsymbol{\sigma}_3)\,, \quad \pm 2^{-\frac{1}{2}}i(\pm\boldsymbol{\sigma}_3 \pm \boldsymbol{\sigma}_1)$$

$$\pm i\boldsymbol{\sigma}_1\,, \pm i\boldsymbol{\sigma}_2\,, \pm i\boldsymbol{\sigma}_3\,, \pm 1\,.$$

(6) $\mathbf{b}$, $\mathbf{c}$, $\mathbf{babab}$

(8) $\{1|\mathbf{a}\}^{-1} = \{1|-\mathbf{a}\},\ \{1|\mathbf{a}\}^{-2} = \{1|-\mathbf{a}\}^{-2} = \{1|-2\mathbf{a}\},\ \{1|\mathbf{a}\}^{0} = \{1|\mathbf{0}\}$