Point Groups and Space Groups in Geometric Algebra

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Abstract. Geometric algebra provides the essential foundation for a new approach to symmetry groups. Each of the 32 lattice point groups and 230 space groups in three dimensions is generated from a set of three *symmetry vectors*. This greatly facilitates representation, analysis and application of the groups to molecular modeling and crystallography.

1. Introduction

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.

A geometric figure or a rigid body is said to be "symmetrical" if there exist 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 such isometries, known as the *Euclidean group* $E(3)$. As is well known, every symmetry $\mathcal{S}$ can be given the mathematical form

$$\mathcal{S} : \mathbf{x} \longrightarrow \mathbf{x}' = \underline{R}\,\mathbf{x} + \mathbf{a}, \tag{1}$$

where $\mathbf{x}$ designates a point in the object, $\underline{R}$ is an orthogonal transformation with the origin as a fixed point, and the vector $\mathbf{a}$ designates a translation.

In most applications the operator $\underline{R}$ is represented by a matrix $[\underline{R}]$, so composition of transformations is achieved by matrix multiplication. This practice has two drawbacks, however. First, use of matrices requires introducing a coordinate system, and that brings in arbitrary features that complicate problems. Second, matrix elements are usually difficult to interpret geometrically. Geometric algebra avoids these drawbacks with the coordinate-free canonical form

$$\underline{R}\,\mathbf{x} = \pm R^\dagger \mathbf{x} R, \tag{2}$$

where R is an invertible multivector, called a *versor*, with even (odd) parity corresponding to the plus (minus) sign. The versor in (2) has been normalized to unity, so its reverse $R^\dagger$ is equal to its inverse R^{-1}. When R is even, equation (2) describes a rotation, and R is often called *rotor* or a *spinor*.

The reader is presumed to be familiar with equation (2) and the versor representation of orthogonal transformations; the subject has been thoroughly treated in (Hestenes 1986) with many applications to mechanics. Surprisingly, this approach has not heretofore been been applied to a systematic treatment of discrete symmetry groups in the published literature. To rectify that deficiency is the first of two major objectives for this paper.

The first half of the paper provides a complete treatment of the *point groups* in two and three dimensions. As this material is not to be found elsewhere, the main ideas are illustrated with examples, and subtle points that are easily overlooked are thoroughly discussed. Aside from the mathematical definition of a group, no prior knowledge about group theory is presumed. The main result is that each of the point groups in three dimensions can be generated from a set of at most three *symmetry vectors* that are tied directly to features of the object. This leads to a new systematic notation and classification scheme for symmetry groups from which one can directly write down the generators for any point group.

The point groups determine the classes of mathematically possible lattices known as *crystal systems*, as explained in Section 4. This shows how geometric algebra can simplify theoretically crystallography

considerably – for the symmetry vectors generating the point group can be identified with *lattice vectors* that generate the lattice. In other words, the point group can be generated multiplicatively from the objects on which it operates. Contrast this with the usual approach which develops the group elements and the lattice as separate entities related only indirectly.

The point group of a lattice leaves a lattice point fixed. To get the complete symmetry group of a lattice, one needs to combine the point group with translations. This raises another problem with the standard representation for a symmetry by (1), namely: The orthogonal group is multiplicative while the translation group is additive, so combining the two destroys the simplicity of both. The source of this problem can be traced to the fact that equation (1) singles out one point, the origin, for special treatment. The second major objective of this paper is to show how geometric algebra provides an elegant solution of this problem with a simple new multiplicative representation for the space groups generated directly from lattice vectors. Sections 4 and 5 introduce the essential mathematical apparatus to achieve this objective.

Section 5 introduces a new homogeneous formulation of Euclidean geometry that treats all points equally and generates an algebra of points, lines and planes. The formalism is applied in Section 6 to create the desired multiplicative model of the Euclidean group. This model provides a precise algebraic formulation of the geometric notion that all symmetries can be generated from reflections in planes. Thereby, it provides a new algebraic foundation for geometric intuition and a powerful tool for computational geometry.

The rest of the paper is devoted to a systematic presentation of generators for the 230 space groups. Although space limitations preclude treatment of all the groups, we do show how to construct any of the generators from symmetry vectors, and we introduce a new scheme of space group symbols that facilitates construction of group generators. All this is illustrated in a complete treatment of the 17 planar space groups.

The techniques and results in this paper hold great promise for simplifying and enriching the use of symmetry groups in crystallography and molecular modeling. There are many fine books on crystallography (O'Keefe and Hyde 1996) that can serve as a guide to practical applications of the method. For an exhaustive description of the 230 space groups, the standard reference is the *International Tables for X-Ray Crystallography* (1992). It is widely used in material science to characterize complex crystal structures, for which the identification of the symmetry, class and space group continues to be a nontrivial task. The International Tables are huge and cumbersome, so the simplifications offered here would be of great value in material science research and engineering. Moreover, the method has potential for much wider application.

2. Point Groups in Two Dimensions

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 $\underline{R}$ taking each vertex $\mathbf{x}_k$ into its neighbor $\mathbf{x}_{k+1}$ as described by

$$\mathbf{x}_{k+1} = \underline{R}\,\mathbf{x}_k = R^\dagger\,\mathbf{x}_k R = \mathbf{x}_k R^2\,. \tag{3}$$

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

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

This relation implies that the "powers" of $\underline{R}$ compose a group with six distinct elements $\underline{R}$, $\underline{R}^2$, $\underline{R}^3$, $\underline{R}^4$, $\underline{R}^5$, $\underline{R}^6 = 1$. 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 $\underline{R}$ is said to be a *generator*

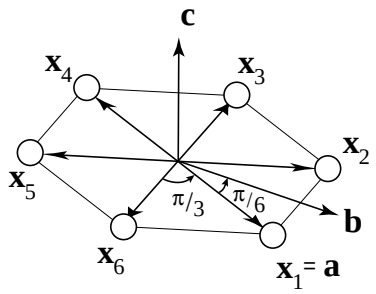


Fig. 1. Planar benzene (C_6H_6), showing generators of the symmetry group. (Hydrogen atoms not shown.)

of $\mathcal{C}_6$, because the entire group can be generated from $\underline{R}$ by the group operation. The group $\mathcal{C}_6$ is completely determined by the condition $\underline{R}^6 = 1$ on its generator, with the tacit understanding that lower powers of $\underline{R}$ 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 $\underline{R}^6 = 1$. It is computationally advantageous to represent rotations by versors rather than linear operators, so we look for a representation of $\mathcal{C}_6$ by versors. According to (3), the operator $\underline{R}$ corresponds to a unique versor $S = R^2$, so the operator relation $\underline{R}^6 = 1$ corresponds to the versor relation

$$S^6 = 1\,. \tag{5}$$

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

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

where $\mathbf{i}$ is the unit bivector for the plane of rotation. The representation (6) shows explicitly that the generator of $\mathcal{C}_6$ is a rotation through angle $\pi/3$.

Now, we know from equation (2) that to every rotation there corresponds two rotors differing only by a sign. Consequently, to every finite rotation group there corresponds a rotor group with twice as many elements. In the present case the generator R of the rotor 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

$$R^6 = -1\,. \tag{7}$$

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 versors. Since the dicyclic group presented by (7) is the versor 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 first explained in (Hestenes, 1986), the pair of rotors $\pm R$ 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.

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 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

$$\underline{A}\mathbf{x} = -\mathbf{a}^{-1}\mathbf{x}\mathbf{a}\,, \tag{8}$$

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

$$\underline{B}\mathbf{x} = -\mathbf{b}^{-1}\mathbf{x}\mathbf{b}\,, \tag{9}$$

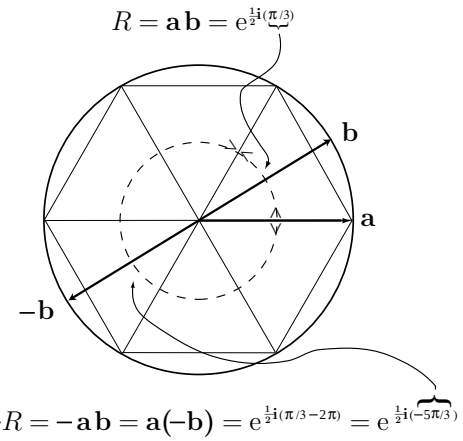


Fig. 2. Illustrating the interpretation of the spinors $\pm R = \pm\mathbf{a}\mathbf{b} = \mathbf{a}(\pm\mathbf{b})$ as equivalent rotations with opposite sense generated by reflections with different senses.

where $\mathbf{b}$ is directed towards the midpoint of a side adjacent to the vertex, as 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

$$\underline{B}\,\underline{A}\mathbf{x} = (\mathbf{a}\,\mathbf{b})^{-1}\mathbf{x}(\mathbf{a}\,\mathbf{b}) \tag{10}$$

is a rotation; in fact, it is the rotation $\underline{R}$ 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

$$\underline{A}^2 = \underline{B}^2 = (\underline{B}\,\underline{A})^6 = 1 \tag{11}$$

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

The rotor 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 (7), the presentation of $2\mathcal{H}_6$ is the set of relations

$$\mathbf{a}^2 = \mathbf{b}^2 = 1\,, \tag{12}$$

$$(\mathbf{a}\,\mathbf{b})^6 = -1\,. \tag{13}$$

According to (9), the two vectors $\pm\mathbf{b}$ in $2\mathcal{H}_6$ correspond to the single reflection $\underline{B}$. Physically, however, one can 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 $\underline{B}$ in (9) 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 (12) and (13). 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 versor 1, as indicated in Table 1. So the versor $1 = e^{\frac{1}{2}\mathbf{i}0}$ represents a rotation of zero angle in the positive sense, while the versor $-1 = e^{-\mathbf{i}\pi} = e^{\frac{1}{2}\mathbf{i}(-2\pi)}$ represents a rotation of 2π with the opposite sense.

Six distinct rotations with "positive sense" represented by	Six distinct rotations with "negative sense" represented by	Twelve distinct reflections represented by
$1 = \mathbf{a}^2 = \mathbf{b}^2$	$-1 = (\mathbf{ab})^6 = (\mathbf{ba})^6$	$\pm\mathbf{a}$
$\mathbf{ab}$	$-\mathbf{ab} = \mathbf{ab}(\mathbf{ba})^6 = (\mathbf{ba})^5$	$\pm\mathbf{aba}$
$(\mathbf{ab})^2$	$-(\mathbf{ab})^2 = (\mathbf{ba})^4$	$\pm\mathbf{ababa} = \pm\mathbf{a}(\mathbf{ba})^2$
$(\mathbf{ab})^3$	$-(\mathbf{ab})^3 = (\mathbf{ba})^3$	$\pm\mathbf{b}$
$(\mathbf{ab})^4$	$-(\mathbf{ab})^4 = (\mathbf{ba})^2$	$\pm\mathbf{bab}$
$(\mathbf{ab})^5$	$-(\mathbf{ab})^5 = \mathbf{ba}$	$\pm\mathbf{babab} = \pm\mathbf{b}(\mathbf{ab})^2$

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

Ordinarily, the group $\mathcal{H}_6$ is regarded as the symmetry group of a regular hexagon. But we have seen that the corresponding versor 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 versor 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*

$$(\mathbf{a}\,\mathbf{b})^p = -1\,, \tag{14}$$

where p is a positive integer. The vectors $\mathbf{a}$ and $\mathbf{b}$ determine reflections (8, 9) which generate the reflection group $\mathcal{H}_p$. The dicyclic group $2\mathcal{C}_p$ is a subgroup of $2\mathcal{H}_p$ generated by

$$\mathbf{a}\,\mathbf{b} = e^{\mathbf{i}\pi/p} = e^{\frac{1}{2}\mathbf{i}(2\pi/p)} \tag{15}$$

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

The versor 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 $p = 1$, (15) 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. 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 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. Note that a reflection will reverse the orientation, so $O(2)$ is the group of an unoriented circle. Note further, 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.

3. 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*

$$(\mathbf{ab})^p = (\mathbf{bc})^q = (\mathbf{ac})^r = -1\,, \tag{16}$$

where p, q, and r are positive integers. If $r = 1$, then (16) implies $\mathbf{c} = -\mathbf{a}$, and $p = q$, so (16) 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 (16) are not independent, for they are related by the equation

$$(\mathbf{ab})(\mathbf{bc}) = \mathbf{ac}\,. \tag{17}$$

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 p, q, and r in (16). The precise nature of the restriction can be ascertained by writing (16) in the equivalent form

$$\begin{aligned} \mathbf{ab} &= e^{i\mathbf{c}'\pi/p}, \\ \mathbf{bc} &= e^{i\mathbf{a}'\pi/q}, \\ \mathbf{ac} &= e^{i\mathbf{b}'\pi/r}. \end{aligned} \tag{18}$$

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 (18) 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, according to the "spherical excess formula" (Hestenes 1986), the area Δ' of the polar triangle is given by

$$\Delta' = \pi\big(\frac{1}{p} + \frac{1}{q} + \frac{1}{r} - 1\big)\,. \tag{19}$$

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

From (19) we can determine the permissible values of p, q, and r. Since the area Δ' must be positive, equation (19) gives us the inequality

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

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 (20) reduces to

$$\frac{1}{p} + \frac{1}{q} > \frac{1}{2}\,. \tag{21}$$

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 (16), 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

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

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

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

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 (16), we get subgroups of $[pq]$ by taking the various poducts of the vectors **a**, **b**, **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 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 can 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. 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. 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

Symbol		Name	Order
Geometric	Schoenflies		
$\overline{\mathrm{p}}$	$\mathcal{C}_p$	(di)cyclic	(2)p
p	$\mathcal{C}_{pv} = \mathcal{H}_p$		(2)2p
$\overline{\mathrm{p2}} = \overline{(2\mathrm{n})2}$	$\mathcal{S}_p$		(2)p = (2)2n
$\overline{\mathrm{p}}\,\overline{2}$	$\mathcal{D}_p$	(di)dihedral	(2)2p
$\mathrm{p}\overline{2} = (2\mathrm{n})\overline{2}$	$\mathcal{D}_{nd}$		(2)2p = (2)4n
$\overline{\mathrm{p}}2$	$\mathcal{C}_{pv}$		(2)2p
p2	$\mathcal{D}_{ph}$		(2)4p
$\overline{3}\,\overline{3}$	$\mathcal{T}$	(di)tetrahedral	(2)12
$33 = \overline{3}3$	$\mathcal{T}_d$		(2)24
$4\overline{3}$	$\mathcal{T}_h$		(2)24
$\overline{4}\,\overline{3}$	$\mathcal{O}$	(di)octahedral	(2)24
$43 = \overline{4}3$	$\mathcal{O}_h$		(2)48
$\overline{5}\,\overline{3}$	$\mathcal{I}$	(di)icososahedral	(2)60
53	$\mathcal{I}_h$		(2)120

Table 3. The (double) point groups in $\mathcal{E}^3$. As indicated by parentheses in the table, for oriented point groups the order is double and the prefix "di" is added to the name for the corresponding orthogonal groups. The groups $\overline{p2}$ and $p\overline{2}$ exist only for values of p, as indicated in the table by writing $p = 2n$, where n is a positive integer. The symbols $\overline{33}$, $\overline{43}$, $\overline{53}$ do not appear, because they do not describe realizable symmetry groups.

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 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.

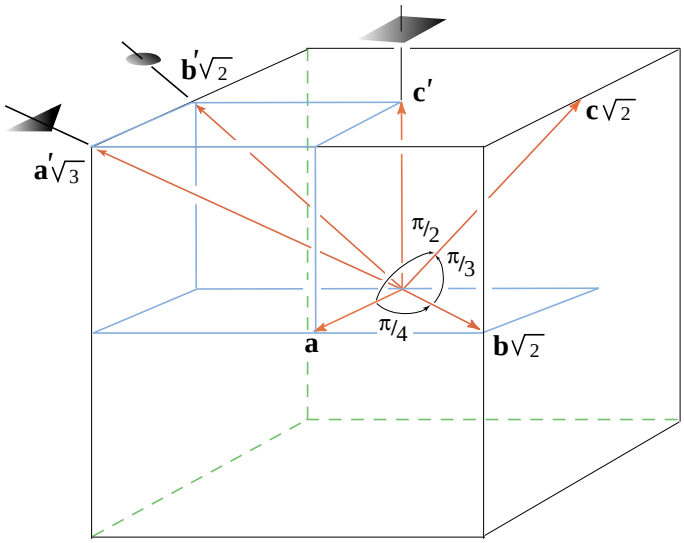


Fig. 3. Generators **a**, **b**, **c** for the double point group [43] of a cube or an octagon. Vertices **a**′, **b**′, **c**′ of the polar triangle (or fundamental region) specify axes of threefold, twofold, and fourfold symmetry, as indicated by the triangle, lense, and square symbols.

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 combinations of rotations and reflections. Some of the mixed groups are identical to reflection groups. For example, the equivalence $43 = \overline{4}3$ means that **a**, **b**, **c** generate the same group as **ab**, **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 **abc**. Since **ab** represents a rotation and **c** represents a reflection, the product **abc** represents a combined rotation and reflection, that is, a rotary-reflection. The quantity $R = (\mathbf{abc})^2$ is an even versor 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 **c** is orthogonal to both vectors **a** and **b**, hence **abc** = **cab** and

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

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

$$R^p = (\mathbf{abc})^{2p} = (\mathbf{ab})^{2p}. \tag{23}$$

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 **a** and **b** is $\pi/4$, the angle between **b** and **c** is $\pi/3$, and the angle between **a** and **c** is $\pi/2$. Figure 3 shows three such vectors in relation to a cube whose reflection group they generate. According to (18), the algebraic relations among the generators are fully expressed by the equations

$$\mathbf{ab} = e^{i\mathbf{c}'\pi/4}, \tag{24}$$

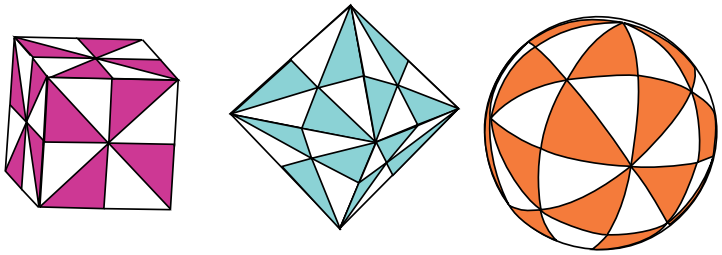


Fig. 4. Fundamental regions for the reflection group $43 = O$ on the surface of a cube, an octagon, or a sphere.

$$\mathbf{bc} = e^{i\mathbf{a}'\pi/3}, \tag{25}$$

$$\mathbf{ac} = e^{i\mathbf{b}'\pi/2} = i\mathbf{b}'\,. \tag{26}$$

The poles $\mathbf{a}'$, $\mathbf{b}'$, $\mathbf{c}'$ are also shown in Fig. 3, It should be evident from Fig. 3 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. 3 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

$$\mathbf{b}' = (\mathbf{ba})^2\mathbf{c}(\mathbf{ab})^2\,. \tag{27}$$

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

$$\mathbf{c}' = (\mathbf{cb})\mathbf{a}(\mathbf{bc}) = \mathbf{cbabc}\,. \tag{28}$$

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. 3. 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, as seen in Fig. 3. 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. 4, so that any operation of the group 43 simply permutes the triangles. Fig. 4 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.

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. 4 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 (19), 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 (19), we find that the orders of the reflection groups $p3$ are given by

$$\frac{4\pi}{\delta'} = \frac{2p}{6-p}\,. \tag{29}$$

This is twice the order of the rotation groups $\bar{p}\overline{3}$, 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.

4. 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 discrete set of points generated by three linearly independent vectors $\mathbf{a}_1$, $\mathbf{a}_2$, $\mathbf{a}_3$. These vectors (and their negatives $-\mathbf{a}_1$, $-\mathbf{a}_2$, $-\mathbf{a}_3$) generate a discrete group under addition known as the *translation group* of the lattice. Each element can be associated with a lattice point designated by $\mathbf{a}_n$ and can be expressed as a linear combination of the generators with integer coefficients, that is,

$$\mathbf{a}_n = n_1\mathbf{a}_1 + n_2\mathbf{a}_2 + n_3\mathbf{a}_3\,, \tag{30}$$

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, we 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 $\{\mathbf{a}_k^*\}$. Although reciprocal frames are familiar tools in crystallography, it is worth mentioning that geometric algebra facilitates their definition and use (Hestenes 1986, Hestenes and Sobczyk 1984). Presently, all we need are the relations

$$\mathbf{a}_j^* \cdot \mathbf{a}_k = \delta_{jk}\,, \tag{31}$$

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

Now, any fixed-point symmetry $\underline{R}$ of a lattice transforms lattice points $\mathbf{a}_k$ $(k = 1, 2, 3)$ into new lattice points

$$\mathbf{s}_k = \underline{R}\mathbf{a}_k = \sum_j \mathbf{a}_j\, s_{jk}\,, \tag{32}$$

where the matrix elements

$$s_{jk} = \mathbf{a}_j^* \cdot \mathbf{s}_k = \mathbf{a}_j^* \cdot (\underline{R}\mathbf{a}_k) \tag{33}$$

are all integers. Consequently, the trace of this matrix

$$\sum_k s_{kk} = \sum_k \mathbf{a}_k^* \cdot (\underline{R}\mathbf{a}_k) \tag{34}$$

is also an integer. This puts a significant restriction on the possible symmetries of a lattice. In particular, if $\underline{R}$ is a rotation symmetry generating a rotation subgroup, then it satisfies a cyclic condition $\underline{R}^p = 1$, and it rotates the lattice through an angle $\theta = 2\pi/p$. It can be shown that

$$\mathrm{Tr}\,\underline{R} = \sum_k \mathbf{a}_k^* \cdot (\underline{R}\mathbf{a}_k) = 1 + 2\cos\,\theta\,. \tag{35}$$

This has integer values only if

$$\cos\,\theta = 0,\ \pm\tfrac{1}{2},\ \pm 1\,, \tag{36}$$

which has the solutions

$$\theta = 0,\ \frac{\pi}{3},\ \frac{\pi}{2},\ \frac{2\pi}{3},\ \pi,\ \frac{4\pi}{3},\ \frac{3\pi}{2},\ \frac{5\pi}{3},\ 2\pi\,. \tag{37}$$

Table 4. The 32 crystal classes (point groups).

System	Class: Geometric	Class: Schoenflies	Class: International	Order	Number of Space Groups
Triclinic	$\bar{1}$	$\mathcal{C}_1$	1	1	1
	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	$\mathcal{C}_{2v}$	mm2	4	22
	22	$\mathcal{D}_{2h} = \mathcal{V}_h$	mmm	8	28
Tetragonal	$\bar{4}$	$\mathcal{C}_4$	4	4	6
	42	$\mathcal{S}_4$	$\bar{4}$	4	2
	$\bar{4}2$	$\mathcal{C}_{4h}$	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}$2m	8	12
	42	$\mathcal{D}_{4h}$	4/mmm	16	20
Trigonal	$\bar{3}$	$\mathcal{C}_6$	3	3	4
(Rhombohedral)	62	$\mathcal{S}_6 = \mathcal{C}_{3i}$	$\bar{3}$	6	2
	$\bar{3}2$	$\mathcal{D}_3$	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
	$33 = \bar{3}3$	$\mathcal{T}_d$	$\bar{4}$3m	24	6
	$43 = \bar{4}3$	$\mathcal{O}_h$	m3m	48	10
					230

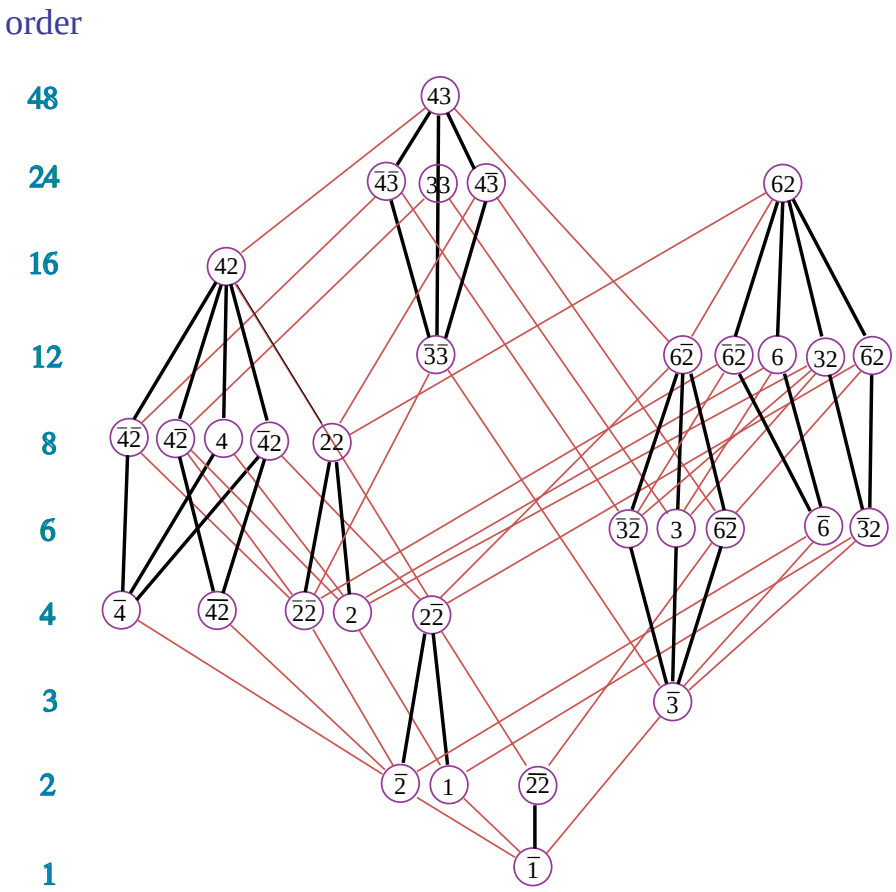


Fig. 5. Subgroup relations among the 32 crystallographic point groups. Dark lines connect groups in the same crystal system.

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

$$p = 1,\ 2,\ 3,\ 4,\ 6\,. \tag{38}$$

This is known as the *crystallographic restriction*.

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* (1992), 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. 5. 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. 6. From the symbols, it is easy to produce a set of generators for each of the seven *diholohedry* (the versor groups of the holohedry). Figure 7 has sets of such generators arranged to show the simple relations among them. Note that the orthogonal vectors **a**, **c** can be chosen to be the same for each system, and there are three distinct choices for the remaining vector **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. 5.

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

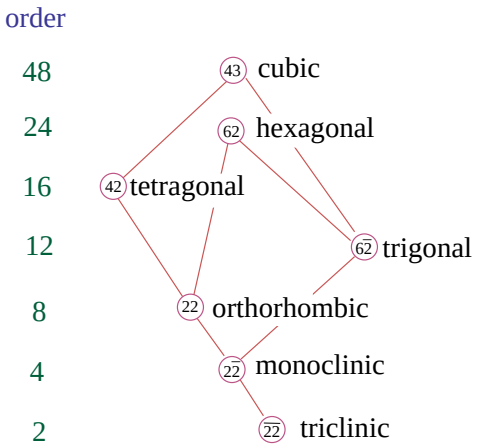


Fig. 6. Subgroup relations for the seven holohedry.

describes a relation among identical parts of an object without saying anything about the nature of those parts.

5. Homogeneous Euclidean Geometry

As an arena for Euclidean geometry we employ the metric vector space $\mathcal{R}^{4,1}$ with *Minkowski signature* (4,1) and its geometric algebra $\mathcal{R}_{4,1} = \mathcal{G}(\mathcal{R}^{4,1})$. The Minkowski signature implies the existence of a cone of null vectors similar to the light cone in spacetime. A vector x is said to be a *null vector* if $x^2 = x \cdot x = 0$. The set of all null vectors in $\mathcal{R}^{4,1}$ is called a *null cone*. Remarkably, the 3d Euclidean space $\mathcal{E}^3$ can be identified with the set of all null vectors in $\mathcal{R}^{4,1}$ satisfying the constraint

$$x \cdot e = 1, \tag{39}$$

where e is a distinguished null vector called the *point at infinity*. This constraint is the equation for a *hyperplane* with normal e. Thus, we identify $\mathcal{E}^3$ with the intersection of a hyperplane and the null cone in $\mathcal{R}^{4,1}$, as expressed by

$$\mathcal{E}^3 = \{x \,|\, x^2 = 0,\ x \cdot e = 1\}, \tag{40}$$

where each x designates a *point* in $\mathcal{E}^3$. This is called the *homogeneous model* of $\mathcal{E}^3$, because all points are treated equally. In contrast, the usual representation of Euclidean points in $\mathcal{R}^3 = \mathcal{R}^{3,0}$ is an *inhomogeneous model* of $\mathcal{E}^3$, because it singles out one point, the *origin*, as special.

The great advantage of the homogeneous model is the simplicity and fluidity that geometric algebra gives to the relations, constructions and inferences of Euclidean geometry. For use in crystal geometry we record some of the basic definitions and results without elaboration. More details are given in (Hestenes 2002, 2001 and 1991), including proofs of some results that are just stated here.

The primary fact is that the squared *Euclidean* distance between any two points x and y is given by

$$(x - y)^2 = -2x \cdot y \tag{41}$$

Thus, Euclidean distances can be computed directly from inner products between points. The *oriented line* (or *line segment*) determined by two distinct points p and q is represented by the trivector

$$P = p \wedge q \wedge e, \tag{42}$$

known as a *line vector* or *sliding vector* in classical parlance. All geometric properties of the line (segment), including its relation to other lines, points and planes, can be computed from trivector P by algebraic means. The *tangent vector* n for the line is

$$n \equiv (p \wedge q) \cdot e = p - q\,. \tag{43}$$

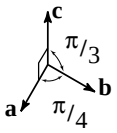
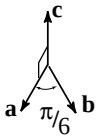
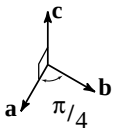
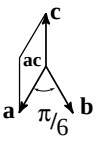
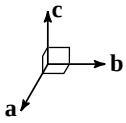
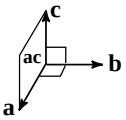
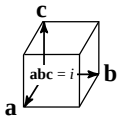
System	Diholohedry	Generators
Cubic	[43]	
Hexagonal	[62]	
Tetragonal	[42]	
Trigonal	$[6\overline{2}]$	
Orthorhombic	[22]	
Monoclinic	$[2\overline{2}]$	
Triclinic	$[\overline{2}\overline{2}]$	

Fig. 7. Generators for the seven diholohedry. One of the generators of $[2\overline{2}]$ and $[6\overline{2}]$ is a bivector $\mathbf{ac}$, and the generator of $[\overline{2}\overline{2}]$ is the unit trivector $\mathbf{abc} = i$. All other generators are vectors.

and the *length* of the line segment is given by

$$P^2 = n^2 = (p - q)^2 = -2p \cdot q. \tag{44}$$

A point x lies on the line P if and only if

$$x \wedge P = x \wedge p \wedge q \wedge e = 0. \tag{45}$$

This is a non-parametric equation for the line.

To relate our homogenous method to the vast literature on geometry and mechanics, we need to relate our homogeneous model for $\mathcal{E}^3$ to the standard vector space model. Happily, this can be done in a straightforward way with an elegant device called the *conformal split*. The essential idea is to parametrize all the points in Euclidean space by the family (or pencil) of lines through a single point.

The *pencil of lines* through a *fixed point* e_0 can be characterized by the variable line vector

$$\mathbf{x} = x \wedge e_0 \wedge e = x \wedge E. \tag{46}$$

This can be inverted to express x as a function of $\mathbf{x}$:

$$x = \mathbf{x}E - \tfrac{1}{2}\mathbf{x}^2 e + e_0, \tag{47}$$

where

$$E \equiv e_0 \wedge e \quad \Longrightarrow \quad E^2 = 1. \tag{48}$$

Thus, we have a one-to-one correspondence between Euclidean points and line segments attached to a given point.

The line vectors specified by (46) form a 3-dimensional vector space

$$\mathcal{R}^3 = \{\mathbf{x}\}, \tag{49}$$

which can be identified with the standard vector space model of $\mathcal{E}^3$, wherein the distinguished point e_0 is represented by the zero vector. The mapping of Euclidean points onto vectors in $\mathcal{R}^3$ defined by (46) and (47) is called a *conformal split*. The conformal split of Euclidean points generates a split of the entire geometric algebra into a commutative product of subalgebras:

$$\mathcal{R}_{4,1} = \mathcal{R}_3 \otimes \mathcal{R}_{1,1}, \tag{50}$$

where $\mathcal{R}_3 = \mathcal{G}(\mathcal{R}^3)$ as before, and $\mathcal{R}_{1,1}$ is the Minkowski geometric algebra generated by the vectors e_0 and e. The chief use of the conformal split is to relate homogeneous geometry to standard vector space geometry. In particular, it enables a smooth connection between the inhomogeneous treatment of point groups in the first part of this paper and the homogeneous treatment of the crystallographic groups in the second.

Two points determine a plane as well as a line. For distinct points p and q with $n \equiv p - q$, the equation for the *oriented plane* bisecting the line between them is

$$n \cdot x = 0. \tag{51}$$

The plane is the set of all points x that are equidistant from the two points, as expressed by $p \cdot x = q \cdot x$ The direction (sign) of n assigns an orientation to the plane. From (39) it follows that every normal has the property

$$n \cdot e = 0. \tag{52}$$

We adopt this as the defining property of a *normal* (vector), because every vector that has it determines a unique plane defined by equation (51). Every normal determines the location as well as the orientation of the plane. It is not essential to specify the normal as a difference between two points, though it is often useful.

The relation of one plane to another is completely determined by the algebraic properties of their normals without reference to any points. To formalize that fact, it is convenient to define the *meet* $n \vee m$ for planes with normals m and n by

$$n \vee m \equiv n \cdot (mI) = (n \wedge m)I, \tag{53}$$

where I is the unit pseudoscalar for $\mathcal{R}_{4,1}$. The meet determines a line vector representing the intersection of the two planes. Indeed, the right side of (53) expresses the meet as the dual of a bivector, so it is a trivector, as required for a line. The condition for a point x to lie on this line is

$$x \wedge (n \vee m) = [x \cdot (n \wedge m)]I = [(x \cdot n)m - (x \cdot m)n]I = 0. \tag{54}$$

This condition is met if and only if $x \cdot n = x \cdot m = 0$. In other words, x must lie in both planes.

There are three distinct ways that the planes might intersect, depending on the value of $n \wedge m$. If $n \wedge m = 0$ the planes coincides. Otherwise,

$$(n \vee m)^2 = -(n \wedge m)^2 = n^2 m^2 - (n \cdot m)^2 \geq 0. \tag{55}$$

If this quantity is positive, the planes intersect in a finite real line. If it vanishes, the planes are parallel, and we may say that the lines intersect in a line at infinity. The concept of a line at infinity is introduce so we can state without exception that every pair of planes intersect in a unique line. The null case in (55) tells us that the line vector for a line at infinity must be the dual of a null bivector.

6. Symmetries from Reflections

It has been known for more than a century that *every* symmetry in $\mathcal{E}^3$ can be generated from reflections in planes (Coxeter 1971). In particular, any *rotation* about a given line can be reduced to a product of reflections in two planes that intersect in that line, and any *translation* can be reduced to a product of reflections in two parallel planes. At long last, geometric algebra makes it possible to cast this powerful geometric insight into a simple algebraic form the facilitates the composition of symmetries.

By definition, a *symmetry* $\underline{S}$ in $\mathcal{E}^3$ is a transformation that leaves invariant the Euclidean distance between points, expressed by $(x-y)^2 = -2x\cdot y$ in our homogeneous model. Invariance of the inner product $x\cdot y$ is the defining property of orthogonal transformations on the vector space $\mathcal{R}^{4,1}$. It is a general theorem of geometric algebra (Hestenes 1991, Hestenes and Sobczyk 1984) that every such transformation $\underline{S}$ taking a generic point x_0 to the point x can be expressed in the canonical form

$$x' = \underline{S}\,x = S^{-1}xS^* \tag{56}$$

where S is an invertible multivector in $\mathcal{R}_{4,1}$ and, as before, $S^* = \pm S$ according to the parity of S.

To preserve our definition of homogeneous Euclidean space, the point at infinity must be an invariant of the symmetry, as expressed by

$$S^{-1}eS^* = e \qquad \text{or} \qquad Se = eS^* = \pm eS. \tag{57}$$

Every such versor can be expressed as a product of vectors:

$$S = n_1 n_2 ... n_k, \tag{58}$$

where

$$n_k \cdot e = 0 \qquad \text{or} \qquad n_k e = -e n_k. \tag{59}$$

Moreover, for given S, the n_k can be chosen so that $k \le 5$.

The great power of this theorem is that it reduces the composition of symmetries, as expressed by the operator equation

$$\underline{S}_2\underline{S}_1 = \underline{S}_3, \tag{60}$$

to a geometric product of their corresponding symmetry versors:

$$S_1 S_2 = S_3. \tag{61}$$

Thus, the *Euclidean group* $E(3)$ is reduced to a multiplicative group of versors.

Comparing (59) with (52), we see that every symmetry vector n is a normal for some plane in $\mathcal{E}^3$. It follows that the symmetry

$$\underline{n}x = -n^{-1}xn \tag{62}$$

is a *reflection* in the "*n-plane*." Indeed, if x is any invariant point of the symmetry, then

$$x = -n^{-1}xn, \qquad \text{so} \qquad nx + xn = 2x\cdot n = 0, \tag{63}$$

which is the normal equation for the n-plane.

The composite symmetry $\underline{S} = \underline{m}\underline{n}$ of reflections in two distinct planes is completely characterized by the geometric product mn of their normals. The symmetry $\underline{S}$ can be generated from many different reflections, so it is desirable to express its versor in a *canonical form* independent of the choice of m and n. For simplicity we impose the normalization $n^2 = m^2 = 1$, though we will have good reason to drop that condition later on. In this case, we have the identity:

$$m^2 n^2 = 1(m\cdot n)^2 - (m\wedge n)^2. \tag{64}$$

Also, the versor constraint (57) takes the form

$$(m\wedge n)\cdot e = 0. \tag{65}$$

There are two different cases to consider, as specified by the conditions (55).

When the planes are parallel, we have $(m \wedge n)^2 = 0$, so the constraint (65) allows us to define a vector a by writing

$$ea = e \wedge a = 2m \wedge n. \tag{66}$$

Therefore, the versor $mn = 1 + m \wedge n$ is equivalent to a versor T_a defined by

$$T_a \equiv 1 + \tfrac{1}{2}ae. \tag{67}$$

A little algebra shows that this versor generates a *translation*

$$\underline{T}_a x = T_a^{-1} x \, T_a = x + a. \tag{68}$$

Squaring this equation, we see that

$$a^2 = -2a \cdot x \tag{69}$$

has the same value for every point x. It can be shown that the right side of (68) has a conformal split of the form

$$x + a = (\mathbf{x} + \mathbf{a})E - \tfrac{1}{2}(\mathbf{x} + \mathbf{a})^2 e + e_0, \tag{70}$$

in agreement with the usual representation for a translation in equation (1).

The conformal split of the translation vector in terms of the plane normals is obtained directly from (66):

$$\mathbf{a} = a \wedge E = a \wedge e_0 \wedge e = 2m \wedge n \wedge e_0 = 2[(m \wedge n)e_0]E, \tag{71}$$

where (65) was used to get the form on the right. The magnitude of the translation is therefore

$$|a| = |\mathbf{a}| = 2|(m \wedge n) \cdot e_0|, \tag{72}$$

which holds for any point e_0 chosen as origin. Also, using

$$eE = e = -Ee \tag{73}$$

to show that

$$ea = e\mathbf{a} = \mathbf{a}e = -ae, \tag{74}$$

we can put (67) in the form

$$T_a = 1 + \tfrac{1}{2}ae = 1 - \tfrac{1}{2}\mathbf{a}e \equiv T_{\mathbf{a}}, \tag{75}$$

where, despite the conformal split of vector a, the right side is independent of the choice of origin.

When the two planes intersect, we have $(m \wedge n)^2 < 0$, and the line vector for the intersection is $L = (m \wedge n)I$. If the origin e_0 is chosen to lie on the line, we have

$$e_0 \wedge L = e_0 \cdot (m \wedge n)I = 0, \tag{76}$$

so the normals have the conformal splits $m = \mathbf{m}E$, $n = \mathbf{n}E$, and the symmetry versor

$$mn = \mathbf{mn} \tag{77}$$

has exactly the rotor form that we studied in Sections 2 and 3. Since the choice of e_0 is arbitrary, we can conclude that the symmetry $\underline{m}\,\underline{n}$ is a rotation about the line $L = (m \wedge n)I$ through half the angle between m and n.

One other symmetry of special interest is *space inversion* at a point p, defined by

$$\underline{I}_p x = I_p x I_p, \qquad \text{where} \qquad I_p = (p \wedge e)I = I_p^{*-1}. \tag{78}$$

This is equivalent to reflection in three mutually orthogonal planes at p. Representing inversion by the trivector versor I_p avoids choosing reflecting planes (as done for the triclinic case in Fig. 7).

7. The Space Groups

We have seen that there are 32 point groups that leave some 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 that 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* generated by at most three vectors $\mathbf{a}$, $\mathbf{b}$, $\mathbf{c}$. 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.

For the three symmetry vectors generating a space group, we choose the set $\mathbf{a}$, $\mathbf{b}$, $\mathbf{c}$ used to generate point groups in Section 4, but we adjust their lengths and directions to generate the shortest translations in the lattice compatible with their function as space group generators. Next we use the results of Sections 5 and 6 to express the versor generators of a space group in terms of its symmetry vectors.

Since all lattice points are equivalent, it is convenient to select one of them, say e_0, as the origin for a conformal split and relate the irreducible generators to that point. The symmetry vectors $\mathbf{a}$, $\mathbf{b}$, $\mathbf{c}$ of Section 4 are translated into normal vectors a, b, c for planes through e_0 by the conformal split

$$a = \mathbf{a}E, \qquad b = \mathbf{b}E, \qquad c = \mathbf{c}E. \tag{79}$$

The condition that e_0 is at the intersection of the three planes is

$$a \cdot e_0 = b \cdot e_0 = c \cdot e_0 = 0. \tag{80}$$

In the homogeneous model, reflections are generated by the normals a, b, c rather than $\mathbf{a}$, $\mathbf{b}$, $\mathbf{c}$, and translations are generated by versors $T_a = T_{\mathbf{a}}$, $T_b = T_{\mathbf{b}}$ and $T_c = T_{\mathbf{c}}$, as defined in (75). This makes it possible to compose reflections and translations by versor multiplication. Note that

$$ab = \mathbf{ab}, \tag{81}$$

so a and b generate the same rotations as $\mathbf{a}$ and $\mathbf{b}$.

The magnitude of a is adjusted so that T_a moves each lattice point to the next one in the direction of a. Likewise for b and c. The inverse translation $T_a^{-1} = T_{-a}$ moves the points back. For integer n, an n-fold application of T_a is equivalent to a single translation by n lattice points, as expressed by the equation

$$T_a^n = T_{na}. \tag{82}$$

Actually, this formula holds for any scalar value of n, although it connects lattice points only when n is an integer. We need fractional values for some space groups. In consonance with equation (30), any translation in the space group can be derived from the irreducible translations by

$$T_{(n_1 a + n_2 b + n_3 c)} = T_a^{n_1} T_b^{n_2} T_c^{n_3}, \tag{83}$$

where the n_k are any integers. Now we are prepared for a detailed analysis of the space groups.

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.

7.1 Planar Space Groups

In two dimensions there are 17 space groups. 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 4 crystal systems distinguished by their symmetry vectors a, b in relation to a lattice.

To see how every 2-dimensional space group can be described in terms of two symmetry vectors, let us examine a representative sample of the groups and generators 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.

The space group symbol includes the slash symbol / to distinguish it from the point group symbol and to indicate that translations must be included among the generators. The number of translations that must be included is not specified, as that is easily inferred from the point group. The symbol after the slash indicates some fusion among reflections and primary translations, as explained below.

In the group $\overline{1}/$, the vectors a and b generate translations only. Since the point group $\overline{1}$ contains only the identity element, it does not imply any relation between the directions of the translation vectors, so the lattice they generate is said to be *Oblique*. As shown in Table 5, the group $\overline{1}/$ has four generators: two irreducible translations and their inverses.

In 2d the point group $\overline{2}$ is generated by the bivector $a \wedge b$, which produces a rotation by π in the plane. Note that the group $\overline{2}/$ has only three generators instead of the four in $\overline{1}/$, because the inverse of any translation is generated according to

$$T_a^{-1} = T_{-a} = (a \wedge b)^{-1} T_a (a \wedge b). \tag{84}$$

The symbol 1 indicates that the groups $1/$ and $1/2$ contain a single reflection versor, say a. Since reflection by a is required to leave the lattice invariant, it must transform translation generators into translation generators. By considering the alternatives, one can see that this can be done in the following ways. In the group $1/$, the reflection is along the direction of one of the translations, so the translation can be reversed by

$$a T_a a = a^2 T_{-a} \doteq T_{-a}, \tag{85}$$

where the symbol $\doteq$ indicates equality up to an irrelevant scale factor (a^2 in this case). If the other translation vector b is orthogonal to a, then

$$a T_b a \doteq T_b. \tag{86}$$

Since a and b determine a rectangle, the lattice they generate is said to be *Rectangular*. Another relation of reflection to translations arises in the *Rhombic* case.

The /2 in the groups $1/2$ and $2/2$ and the /3 in $3/3$ indicates a fractional combination of primary translations T_a, T_b. The primary translations can be derived therefrom: for example,

$$(T_{a+b}^{1/3})^2 \; ab \; T_{a+b}^{1/3} \; ba \doteq T_a. \tag{87}$$

Note in Table 5, that the choice of symmetry vectors a, b is different for the group $3/3$ than for the groups $3/$ and $\overline{3}/$, though they pertain to the same lattice.

The $\overline{2}$ in the group symbol $4/\overline{2}$ specifies a reflection-translation combination, such as

$$a T_{a/2} = T_{a/4}^{-1} a T_{a/4}, \tag{88}$$

which represents reflection in a line (or plane in 3d) displaced from the origin by $a/4$. The number 2 specifies the relation

$$(a T_{a/2})^2 \doteq 1, \tag{89}$$

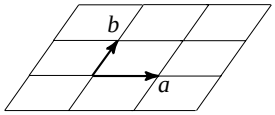
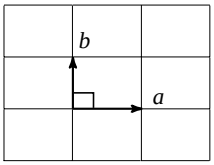
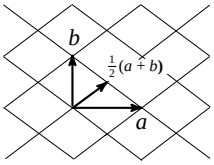
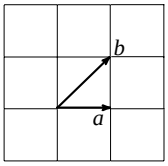
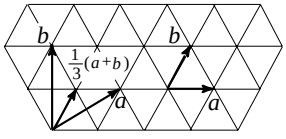
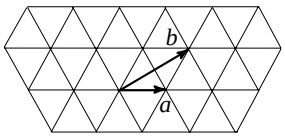
The g in the group symbol $1/g$ designates a *glide-reflection* with a versor generator of the form

$$G = a T_{b/2} = T_{b/2} a, \tag{90}$$

where b must be orthogonal to a. Note that

$$G^2 = a^2 T_{b/2}^2 \doteq T_b, \tag{91}$$

Table 5. The 17 planar space groups.

System and Lattice	Space Group Symbol		Space Group Generators
	Geometric	International	
Oblique 	$\overline{1}/$	p1	$T_{\pm a}, T_{\pm b}$
	$\overline{2}/$	p2	$a \wedge b, T_a, T_b$
Rectangular 	$1/$	pm	$a, T_a, T_{\pm b}$
	$1/\mathrm{g}$	pg	$aT_{\pm b/2}, T_{\pm a}$
	$1/2$	cm	$a, T^{1/2}_{(a \pm b)}$
	$2/$	pmm	a, b, T_a, T_b
Rhombic 	$2/\mathrm{g}$	pmg	$ab, aT_{b/2}, T_a$
	$2/\overline{\mathrm{g}}$	pgg	$ab, aT^{1/2}_{a+b}$
	$2/2$	cmm	$a, b, T^{1/2}_{a+b}$
Square 	$\overline{4}/$	p4	ab, T_a
	$4/$	p4m	a, b, T_a
	$4/\overline{2}$	p4g	$ab, aT_{a/2}$
Trigonal 	$\overline{3}/$	p3	ab, T_a
	$3/$	p3m1	a, b, T_a
	$3/3$	p31m	$a, b, T^{1/3}_{a+b}$
Hexagonal 	$\overline{6}/$	p6	ab, T_a
	$6/$	p6m	a, b, T_a

so T_b is not a primitive generator in this case.

The bar over the g in the group symbol $2/\overline{g}$ indicates a product of fractional translations fused with a reflection to produce a displaced glide-reflection, as in the generator

$$aT^{\frac{1}{2}}_{a+b} = aT_{a/2}T_{b/2} = T^{-1}_{a/4}aT_{b/2}T_{a/4}, \tag{92}$$

which generates a glide-reflection along a line displaced from the origin by $a/4$.

In the group $1/g$ the reflection signified by the symbol 1 is fused with a translation into a glide-reflection. Consequently, the point group 1 is not a subgroup of $1/g$, as it is in $1/$ and $1/2$. For this reason, the symbol 1 is said to specify the *class* rather than the point group of the space groups $1/$, $1/2$ and $1/g$.

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 generating translations. On the other hand, a group like $4/$ has only one lattice constant corresponding to a single generating translation, as all other translations are obtained from the one by operations of the point group.

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 lattice types illustrated in Table 5. It will be noted that two distinct lattice types, the Rectangular and the Rhombic, are derived from the same *system* of generating vectors. As Table 5 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. 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 discussed in many fine books such as (Coxeter 1971).

7.2 3d Space Groups

Generalization of the planar case to get the 230 space groups in $\mathcal{E}^3$ is fairly straightforward. One simply introduces a third symmetry vector c and its translation T_c and considers all possible ways to combine them with the planar generators in Table 5. The task is simplified by the fact that all the planar generators appear also in the 3d space groups without change in form or notation. Some complexity arises from the fact that there are 14 different lattice types in 3d.

All possible relations of vector a to vector b are enumerated in Table 5. Their possible relations to the third vector c are governed by the 3d crystal systems and holohedry in Figs. 6 and 7. From Fig. 7 we see immediately that we can choose c orthogonal to a in every 3d crystal system, and c must then be orthogonal to b in every crystal system except the *Cubic system*.

As an example of how to construct the 3d space groups and generators from the 2d case, note that all the 2d crystal classes 1, $\overline{1}$, 2, $\overline{2}$, 3, $\overline{3}$, 4, $\overline{4}$, 6, $\overline{6}$, appear also as 3d crystal classes in Table 4. Simply by combining T_c (but not c) with all the planar group generators in Table 5, we get all the 3d space groups in those classes. Each of the 17 planar groups branches into several 3d groups depending on how T_c is combined with their generators. The only new kind of generator arising from this is the fusion of T_c with a rotation versor ab to produce a *screw displacement*. To be specific, since c is orthogonal to a and b with

$$(ab)^p = (\mathbf{ab})^p = -1, \tag{93}$$

we can construct a screw displacement versor

$$S = abT^{1/p}_c = T^{1/p}_c ab, \tag{94}$$

with the property

$$S^p = -T_c \doteq T_c. \tag{95}$$

In this case, the screw axis passes through the origin in the direction of c. Note the similarity of the screw equations (94) and (95) to the glide-reflection equations (90) and (91). The screw axis can also be displaced from the origin like it is for a glide-reflection in (92).

In the other 3d space groups the reflection vector c comes into play. However, its fusion with translations to produce new space groups does not differ in any essential way from the cases we have already considered. Of course, in some space groups c is not fused with any translation. The simplest example is the generalization of the 2d space inversion in equation (84) to the 3d space inversion point group $\overline{22}$ generated by the trivector $I_0 = (e_0 \wedge e)I = EI$. This particularizes the general definition of space inversion by (78). The corresponding space group $\overline{22}/$ is the symmetry group for a triclinic lattice.

Note: A patent is pending on application of the homogeneous method to crystallographic modeling and analysis.

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