The Crystallographic Space Groups in Geometric Algebra[1]

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Abstract. We present a complete formulation of the 2D and 3D crystallographic space groups in the conformal geometric algebra of Euclidean space. This enables a simple new representation of translational and orthogonal symmetries in a multiplicative group of versors. The generators of each group are constructed directly from a basis of lattice vectors that define its crystal class. A new system of space group symbols enables one to unambiguously write down all generators of a given space group directly from its symbol.

1. Introduction

Symmetry groups are powerful tools for describing structure in physical systems. For a given system, a *symmetry* is defined mathematically as an invertible mapping of the system onto itself that leaves some property invariant. This article is concerned with the symmetries of molecular configurations, for which the invariants are Euclidean distances between constituent atoms. For molecules of finite extension, the symmetry groups are composed of reflections and rotations with a common fixed point, so they are called *point groups*. Large molecules extended to an infinite periodic lattice have translation symmetries as well. The symmetry groups of such ideal crystals are called (crystallographic) *space groups*. It happens that point symmetries combine with translations in subtle ways to form exactly 17 different 2D space groups and 230 different 3D space groups. This article introduces a new algebraic representation for the space groups, including, for the first time, a complete presentation of the generators for each group in a single table. By "presentation" we mean an explicit representation of group elements. We also introduce a compact new system of space group symbols that enables one to write down the generators for each group directly from the group symbol.

Standard treatments of the space groups are based on the usual representation of points in Euclidean 3-space $\mathcal{E}^3$ by vectors in a real vector space $\mathcal{R}^3$. They begin with the general theorem that every displacement or symmetry $\mathcal{S}$ of a rigid body can be given the mathematical form

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

where $\mathbf{x}$ and $\mathbf{x}'$ designate points, $\underline{R}$ is an orthogonal transformation with the origin as a fixed point, and the vector $\mathbf{a}$ designates a translation. Orthogonal transformations are

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represented by matrices and composed multiplicatively while translations are composed additively. This representation has a number of drawbacks: it is inhomogeneous in the sense that it singles out the origin for special treatment, it intertwines the representation of points and symmetries, and it obscures the relation of translations to point symmetries.

It has been demonstrated recently that all these drawbacks can be eliminated in *Geometric Algebra* (GA) by replacing the standard *vector space model* of $\mathcal{E}^3$ with a homogeneous *conformal model* [1]. The new insights led immediately to a new representation for the space groups within *"conformal"* GA [2]. The present article reviews and completes that work. Although essential features of GA are summarized herein, more extensive background in GA will be helpful to the reader. See [3] for a quick introduction or [4] for a comprehensive treatment. For further analysis of reflection groups that is easily related to the present approach see [5, 6, 7]. As developed here, the space groups are discrete subgroups of the Euclidean conformal group. For treatment of the full conformal group with conformal GA see [8]. Conformal GA has a wide range of applications to physics, engineering and computer science under active investigation. [9, 10]

2. Geometric Algebra

Here we summarize basic features and results of GA needed to characterize the space groups. Supporting proofs and calculations are given in the references.

We begin with the usual notion of a real vector space $\mathcal{R}^{(r,s)}$ of dimension $r+s$, including vector addition, scalar multiplication, and a scalar-valued inner product with signature (r, s). By introducing the *geometric product* of vectors we generate the *geometric algebra* $\mathcal{R}_{(r,s)} = \mathcal{G}(\mathcal{R}^{(r,s)})$. Thus there are many kinds of GA distinguished by dimension and signature. Two signatures are of special interest for modeling the physical space groups: *Euclidean signature* $(r, 0)$ and *Lorentz signature* $(r, 1)$. The latter is familiar for modeling spacetime in the Theory of Relativity, so its use for modeling space groups may come as an amusing if not enlightening surprise. The common features of both cases are elucidated in the general treatment for arbitrary signature in this section.

As in any algebra, the geometric product ab is associative and distributive. However, it is not commutative, and it is related to the usual scalar-valued *inner product* $a \cdot b$ by

$$a \cdot b = \frac{1}{2}(ab + ba). \tag{2}$$

It follows that $a^2 = a \cdot a$ is scalar-valued, so this defines a scalar magnitude $|a|$ for the vector a. There are three cases: the *signature* of a is said to be *positive* if $a^2 = |a|^2$, *negative* if $a^2 = -|a|^2$, or *null* if $a^2 = |a|^2 = 0$.

Taking the geometric product as fundamental, we can regard (2) as a definition of the inner product. Similarly, we can define an *outer product* by

$$a \wedge b = \frac{1}{2}(ab - ba). \tag{3}$$

The two definitions combine to give us the fundamental equation

$$ab = a \cdot b + a \wedge b. \tag{4}$$

Unlike inner and outer products alone, for non-null vectors the geometric product admits a multiplicative inverse given by

$$a^{-1} = \frac{1}{a^2}a = \pm\frac{a}{|a|^2}, \tag{5}$$

where the sign is the vector's signature.

Generic elements in GA are called *multivectors.* By multiplying vectors $a_1, a_2, \ldots, a_k$ we generate a multivector

$$A = a_1 a_2 \cdots a_k. \tag{6}$$

This multivector is said to have *even* or *odd parity* given by the sign of $(-1)^k$. By reversing the order of multiplication we get a different multivector

$$A^\dagger = a_k \cdots a_2 a_1. \tag{7}$$

This operation, called *reversion*, is analogous to hermitian conjugation in matrix algebra. We use it to define a magnitude $|A|$ by

$$|A|^2 = |a_1|^2 |a_2|^2 \cdots |a_k|^2 = \pm A A^\dagger, \tag{8}$$

where the sign is determined by the signature of the vectors.

We can generalize the definition of outer product (3) by antisymmetrizing the product of k vectors and denoting the result by

$$\langle A \rangle_k = a_1 \wedge a_2 \wedge \cdots \wedge a_k. \tag{9}$$

This quantity is called a k-vector, and the notation on the left expresses it as the k-vector part of multivector A. As the notation indicates the outer product is associative, and by definition it is antisymmetric under interchange of any two vectors. It follows that the outer product vanishes if and only if the k vectors are linearly dependent, so the outer product is ideal for expressing linear independence.

If none of the vectors in (6) is null, the multivector A is called a *versor*, and it has a multiplicative inverse

$$A^{-1} = a_k^{-1} \cdots a_2^{-1} a_1^{-1} = \pm \frac{A^\dagger}{|A|^2}, \tag{10}$$

where the sign depends on signature. It follows that any given set of versors generates a multiplicative group, where the group product of versors A and B is simply the geometric product producing a new versor

$$C = AB. \tag{11}$$

Moreover, the versors with even parity form a subgroup.

Now we are equipped to formulate the fundamental theorem from which all our results flow. We think it is one of the most important theorems in all of mathematics, as central to linear algebra as the Pythagorean theorem is to elementary geometry. It is little known and used outside GA, because it takes GA to reveal its simplicity and power. It does not even have a standard name; let us call it the *Versor Theorem* to emphasize the fundamental role of versors.

Recall that an orthogonal transformation on the vector space $\mathcal{R}^{(r,s)}$ is defined as a linear transformation that leaves the inner product invariant. Accordingly, we state the *Versor Theorem: Every orthogonal transformation* $\underline{A}$ *can be expressed in the canonical form*

$$\underline{A} : x \longrightarrow x' = \underline{A}(x) = \pm A^{-1} x A = \pm \frac{A^\dagger x A}{|A|^2}, \tag{12}$$

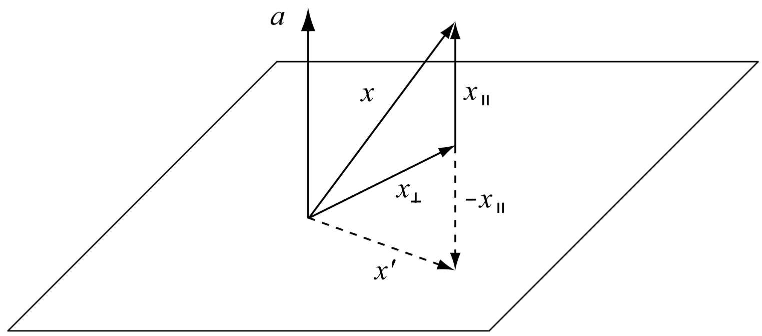

Fig. 1. Reflection of vector x through the plane with normal vector a.

where A is a versor and the sign is its parity. In other words, every versor A determines a unique orthogonal operator $\underline{A}$ given by (12). Conversely, it is obvious that $\underline{A}$ determines A up to an arbitrary sign and scale factor. Hence, the *unit versor* $\hat{A} = A|A|^{-1}$ is a double-valued representation of $\underline{A}$. Though magnitude is irrelevant to versor representation of orthogonal transformations, it is often convenient to work with unnormalized versors, as we shall see, when representing space groups.

The orthogonal transformations on $\mathcal{R}^{(r,s)}$ compose the *orthogonal group* $\mathsf{O(r,s)}$, where the group product is defined by the composition of linear operators. From (12) we see that composition of operators $\underline{A}$ and $\underline{B}$ gives us the new operator

$$\underline{C}(x) = \underline{B}\,\underline{A}(x) = \pm B^{-1}(A^{-1}xA)B = \pm(AB)^{-1}x(AB) = \pm C^{-1}xC, \tag{13}$$

where versor C is given by the geometric product $C = AB$. Factoring out the irrelevant scale factors, we have proved that the unit versors in $\mathcal{R}_{(r,s)}$ compose a double-valued group represention of $\mathsf{O(r,s)}$. This group of unit versors is called the *Pin group* $\mathsf{Pin(r,s)}$ in the mathematics literature. It has the enormous advantage of reducing group composition to simple multiplication of versors. Versor representations are much simpler than the usual matrix group representations, as is obvious in the applications below.

Even versors, that is, versors with even parity form an even subgroup of $\mathsf{Pin(r,s)}$ called $\mathsf{Spin(r,s)}$. This spin group is a double-valued representation of the *special orthogonal group* $\mathsf{SO(r,s)}$, sometimes called the *rotation group* for $\mathcal{R}^{(r,s)}$. In Section 4 we will see how all the 3D space groups can be represented as discrete versor subgroups of $\mathsf{Pin(3+1,1)}$.

The simplest kind of versor is a single vector, and the linear transformation that it generates is called a *reflection.* The reflection generated by vector a has the form

$$\underline{a}\,(x) = -a^{-1}xa = x_\perp - x_\|, \tag{14}$$

where $x_\| = x \cdot aa^{-1}$ is the component of x along a and $x_\perp = x \wedge aa^{-1}$ is the component of x orthogonal to a, as illustrated in Fig. 1.

Every vector a is normal to a hyperplane through the origin determined by the equation $x \cdot a = 0$, a straightforward generalization of the familiar equation for a plane in 3D. For this reason, the reflection (14) is more precisely described as *reflection in a hyperplane* with normal a. Indeed, we can regard every vector a by itself as the versor representation of a reflection without further reference to the hyperplane it determines. Successive reflections are then represented by simply multiplying vectors. From our discussion above, it is obvious that every orthogonal transformation can be generated and represented in this way. Next we turn to practical applications of this result.

3. Point Groups with the Vector Space Model of $\mathcal{E}^3$

With the apparatus of GA well in hand, we now return to the vector space model of $\mathcal{E}^3$, which represents Euclidean points by vectors in $\mathcal{R}^3 = \mathcal{R}^{(3,0)}$. We signify those vectors with boldface letters to distinguish them from the alternative representation by vectors in the conformal model introduced in the next section. As explained elsewhere [3], the geometric algebra $\mathcal{R}_3 = \mathcal{R}_{(3,0)}$ is isomorphic to the familiar Pauli algebra used in quantum mechanics, although its representation by matrices is irrelevant to physical applications, as demonstrated once again in the following.

As we learned in the preceding section, the algebra $\mathcal{R}_3$ enables us to write the orthogonal transformation in (1) in the form

$$\underline{R}\mathbf{x} = \pm R^{-1}\mathbf{x}R, \tag{15}$$

where versor R is an element of $\mathsf{Pin(3)} = \mathsf{Pin(3,0)}$. If R is even, it belongs to $\mathsf{Spin(3)} = \mathsf{Spin(3,0)}$, which is equivalent to the usual spin group in nonrelativistic quantum mechanics. We are interested here only in discrete subgroups that represent symmetries of molecular point groups. Since that subject has been thoroughly covered in [2], we simply state the results we need.

As each point group is uniquely determined by a set of generating versors, we can restrict our attention to the corresponding versor group, which we refer to as a *versor point group*. In 3D every such group can be constructed from a set of three distinct vectors, say $\mathbf{a}$, $\mathbf{b}$, $\mathbf{c}$. As described by (15), each vector generates a reflection in a plane, often called a *mirror reflection* in the crystallographic literature.

The product $\mathbf{ab}$ of two vectors generates a rotation

$$\underline{R}\mathbf{x} = (\mathbf{ab})^{-1}\mathbf{x}(\mathbf{ab}) \tag{16}$$

through twice the angle between $\mathbf{a}$ and $\mathbf{b}$, as shown in Fig. 2. Therefore, the versor $(\mathbf{ab})^p$ generates a rotation through p times that angle. This versor generates a finite rotation

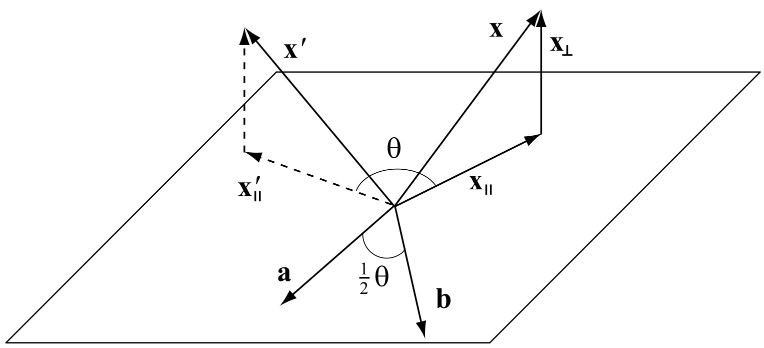

Fig. 2. Rotation of vector $\mathbf{x}$ through the angle θ about an axis perpendicular to vectors $\mathbf{a}$ and $\mathbf{b}$. Note that the rotation is through twice the angle between $\mathbf{a}$ and $\mathbf{b}$.

Crystal System	Point Group	
	International	Geometric
Oblique	1	$\bar{1}$
	2	$\bar{2}$
Rectangular	m	1
	mm	2
Trigonal	3m	3
	3	$\bar{3}$
Square	4m	4
	4	$\bar{4}$
Hexagonal	6m	6
	6	$\bar{6}$

Table 1. The 10 two-dimensional point groups and the crystal systems to which they belong. Both the international and geometric symbols are given for comparison.

group if there is a smallest integer p for which

$$(\mathbf{ab})^p = -|\mathbf{a}|^p|\mathbf{b}|^p \doteq -1, \tag{17}$$

where $\doteq$ means equality modulo a scale factor, which is equivalent to normalizing the versors to unity. This constraint tells us that the angle between $\mathbf{a}$ and $\mathbf{b}$ is $\frac{180^\circ}{p}$. Obviously, the versor group is extended to include reflections simply by adopting the vectors $\mathbf{a}$ and $\mathbf{b}$ as generators.

The possible values of integer p are limited by requiring that the generators are *lattice vectors*. This determines the 10 possible 2D point groups listed in Table 1, where the value of p serves as a *geometric symbol* for the point group generated by reflections and the overbar symbol $\bar{p}$ designates its rotation subgroup. The symbol $p = 1$ designates the case when there is only one vector generator.

The 3D point groups are determined by the following constraints on the generating vectors (see [2] for a complete justification):

$$(\mathbf{ab})^p \doteq (\mathbf{bc})^q \doteq (\mathbf{ca})^2 \doteq -1. \tag{18}$$

One of the rotation angles is restricted to 90° because the three rotation generators are related by

$$(\mathbf{ab})(\mathbf{bc}) = |\mathbf{b}|^2\mathbf{ac} \doteq \mathbf{ac}. \tag{19}$$

Consequently, each point group is determined by values for the two integers p and q and can be designated by the geometric symbol pq with overbars indicating any restrictions to rotation subgroups. The 32 distinct possibilities are listed in Table 2 along with the international symbols for the crystallographic point groups. A summary of how to read off the point group generators from the geometric symbol is given in Table 3.

{A reviewer pointed out that the group notation in Tables 1 and 2 is isomorphic to Coxeter's notation in Table 2 of [7], with the correspondences $q \leftrightarrow [q], \bar{q} \leftrightarrow [q]^+, \overline{pq} \leftrightarrow$

Crystal System	Point Group	
	International	Geometric
Triclinic	1	$\bar{1}$
	$\bar{1}$	$\overline{22}$
Monoclinic	2	$\bar{2}$
	m	1
	2/m	$\bar{2}2$
Orthorhombic	222	$\bar{2}\bar{2}$
	mm2	2
	mmm	22
Tetragonal	4	$\bar{4}$
	$\bar{4}$	$\overline{42}$
	4/m	$\bar{4}2$
	422	$\bar{4}\bar{2}$
	4mm	4
	$\bar{4}$2m	$4\bar{2}$
	4/mmm	42
Trigonal	3	$\bar{3}$
	$\bar{3}$	$\overline{62}$
	32	$\bar{3}\bar{2}$
	3m	3
	$\bar{3}$m	$6\bar{2}$
Hexagonal	6	$\bar{6}$
	$\bar{6}$	$\bar{3}2$
	6/m	$\bar{6}2$
	622	$\bar{6}\bar{2}$
	6mm	6
	$\bar{6}$m2	32
	6/mmm	62
Cubic	23	$\bar{3}\bar{3}$
	m3	$4\bar{3}$
	432	$\bar{4}\bar{3}$
	$\bar{4}$3m	$33 = \bar{3}3$
	m3m	$43 = \bar{4}3$

Table 2. The 32 three-dimensional point groups and the crystal systems to which they belong. Listed are both the international and geometric symbols for the groups.

$[p^+, q^+], \bar{p}q \leftrightarrow [p^+, q], \bar{p}\bar{q} \leftrightarrow [p, q]^+$. The notations were created independently. No doubt their striking similarity is due to building the groups out of reflections, in contrast to other approaches that start with rotations and add reflections afterwards. Note, however, that our notation refers to versor generators, whereas, Coxeter's notation refers to the orthogonal transformations they generate.}

4. The Euclidean Group in Conformal GA

In the conformal model for Euclidean geometry the points of $\mathcal{E}^3$ are identified with null vectors in $\mathcal{R}^{(4,1)}$ and its geometric algebra $\mathcal{R}_{(4,1)}$. Hence each point x satisfies

$$x^2 = 0. \tag{20}$$

One null vector e is singled out as the *point at infinity* so that finite Euclidean points lie in the hyperplane

$$x \cdot e = -1. \tag{21}$$

These two constraints define a 3D paraboloid in a 5D vector space. The remarkable fact is that this surface has a natural Euclidean structure.

Point Group Symbol	Generators
p (=1)	$\mathbf{a}$
p ($\neq 1$)	$\mathbf{a}$, $\mathbf{b}$
$\bar{p}$	$\mathbf{ab}$
pq	$\mathbf{a}$, $\mathbf{b}$, $\mathbf{c}$
$\bar{p}q$	$\mathbf{ab}$, $\mathbf{c}$
$p\bar{q}$	$\mathbf{a}$, $\mathbf{bc}$
$\bar{p}\bar{q}$	$\mathbf{ab}$, $\mathbf{bc}$
$\overline{pq}$	$\mathbf{abc}$

Table 3. Geometric point group symbols and their generators. The angles between the generating vectors are related to p and q as described in the text.

The oriented line segment connecting points x and y is represented by the trivector $x \wedge y \wedge e$, and its length, equal to the Euclidean distance between the points, is given by

$$(x \wedge y \wedge e)^2 = (x - y)^2 = -2x \cdot y. \tag{22}$$

Thus, Euclidean distance is given directly by the inner product between points, which has been made possible by the representation of points as null vectors.

The conformal model is most directly related to the vector space model by designating one point e_0 as the origin and representing the other points by

$$\mathbf{x} \equiv x \wedge e_0 \wedge e = x \wedge E, \tag{23}$$

which, with bivector $E = e_0 \wedge e$ held fixed, defines a mapping into 3D vectors. Equation (23) can be inverted to yield

$$x = \mathbf{x}E - \frac{1}{2}\mathbf{x}^2 e + e_0. \tag{24}$$

It follows that $(x - y)^2 = (\mathbf{x} - \mathbf{y})^2$, so the measure of Euclidean distance between points is the same in both models. That established, we can confidently treat Euclidean geometry in the conformal model without further reference to the vector model. And we are well justified in referring to the algebra $\mathcal{R}_{(4,1)}$ as *conformal GA*.

Every vector in conformal GA represents a significant geometric object, though only null vectors represent Euclidean points. In particular, modulo an arbitrary scale factor, each vector a orthogonal to the point at infinity represents a unique (oriented) plane in $\mathcal{E}^3$. The sign of a specifies orientation, which we often ignore. The equation for the a-plane has the familiar form

$$x \cdot a = 0. \tag{25}$$

In the vector space model an equation of this form holds only for planes through the origin. Remarkably, however, it applies to every plane in the conformal model. To see how that works, suppose that $2a$ is the displacement vector between two points p and q defined by $2a = p - q$. Then $2e \cdot a = e \cdot p - e \cdot q = 0$, as required for a plane. And, according to (22), $2x \cdot a = x \cdot p - x \cdot q = 0$ tells us that all points on the plane are equidistant from p and q.

Thus, we can regard a as the displacement from the plane to the point p or from the point q to the plane. To emphasize the fact that this displacement is along a line normal to the plane, we could call it a *normal displacement.* Actually, as is evident in the next paragraph, the displacement is not from a plane to a point but to a parallel plane through that point.

Let us refer to a as the *normal* of the a-plane, but take note that, unlike the usual notion of "normal," it specifies the location of the plane as well as its direction and orientation. Indeed, we can regard a as a complete algebraic representation of the plane, as it determines all properties of the plane uniquely. We can also regard it as a versor representation of reflection in the plane, as specified by eqn. (14). The transformation group generated by all such *normal reflections* is the *Euclidean group* $\mathsf{E}(3)$. Conversely, every operator in $\mathsf{E}(3)$ has a simple versor representation as a product of normals. The great advantage of this representation is that both translations and rotations are represented by versor products.

It is well known that every rotation can be expressed as a product of reflections in two planes intersecting along the rotation axis, and every translation can be expressed as a product of reflections in two parallel planes separated by half the length of the translation (see Chaps. 2,3 & 7 of [6]). Conformal GA makes it possible to express these simple geometric facts as simple geometric products of the plane normals. In the conformal model the versor representation of a rotation as a product ab is essentially the same as in the vector space model described in the previous section, except that the reflection planes were tied to the origin there. The versor representation of translations is a bit different.

If m and n are unit normals for parallel planes, we can define a vector a by $ae = 2m \wedge n$ so the translation versor can be put in the form

$$mn \;= 1 + m \wedge n = 1 + \frac{1}{2}ae \equiv T_a. \tag{26}$$

A little algebra shows that this versor generates the translation

$$x' = \underline{T}(x) = T_a^{-1} x T_a = x + a + \frac{1}{2}(x+a)^2 e, \tag{27}$$

where the last term is a scaling at infinity insuring that translated points remain null. [11] That term is eliminated in $x' \wedge e = x \wedge e + a \wedge e$. "Wedging" this with an arbitrary point e_0 chosen for an origin and using (23), we demonstrate equivalence to the usual equation for a translation in the vector space model

$$\mathbf{x}' = \mathbf{x} + \mathbf{a}. \tag{28}$$

Now compare the *translation vector* in eqn. (27) with the *displacement vector* determining the bisecting plane defined by eqn. (25). They differ only in their components at infinity; therefore they project to the same 3-space vector $\mathbf{a}$ as in eqn. (28), and their depictions in spatial figures will be the same. Their difference actually has geometric significance, but that is not relevant to our present concerns. The most important point here is that the translation versors form a multiplicative group with composition law $T_a T_b = T_{a+b}$ and inverse $T_a^{-1} = T_{-a}$, so n-fold powers can be expressed by $T_a^n = T_{na}$. Thus, we see how the additive group of displacements is mapped into a multiplicative group of versors.

Now we have all the mathematics we need for a conformal treatment of the space groups. But first, let's place it in a more general context. The adjective "conformal" comes from the established term *conformal mapping* for angle-preserving mappings on Euclidean space.

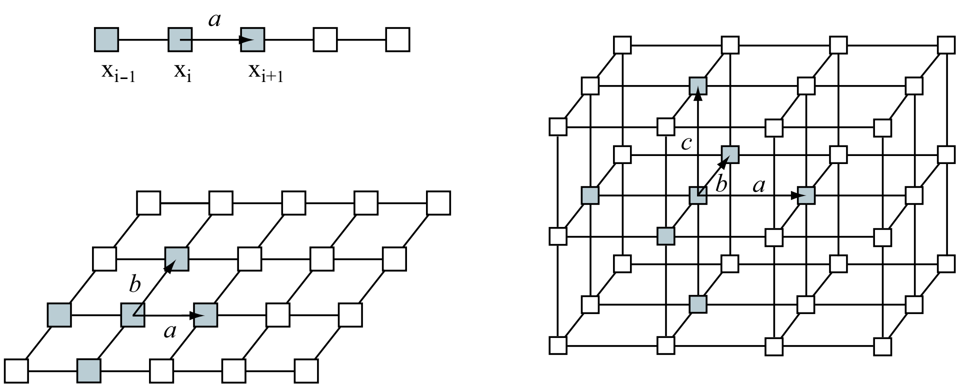

Fig. 3. Examples of one-, two-, and three-dimensional lattices and their lattice vectors. The lattice vectors are given by one-half the distance between neighboring sites (shaded), so that in the one-dimensional lattice we have $a = \frac{1}{2}(x_{i+1} - x_{i-1})$.

The group of such mappings on the vector space $\mathcal{R}^{(r,s)}$ is called the *conformal group* C(r,s). It has been known for a long time that this group is isomorphic to the orthogonal group O(r+1,s+1), but the practical significance of this fact has been recognized only recently [1]. In the conformal model for $\mathcal{E}^3$ the conformal group is equivalent to O(4,1). We are interested here only in the *Euclidean group* E(3), which is the subgroup of O(4,1) that leaves the point at infinity invariant. The versor representation of E(3) does not have a name, but it is so important that it deserves one, so let's call it the *Euclidean Pin group* E-Pin(3). The versor space groups are all discrete subgroups of this group. Our next task is to construct them.

5. Space Groups in Conformal GA

Construction of the space groups begins with a few basics facts about crystal lattices that are established in the many good books on crystallography [13, 14, 15]. In the conformal model, lattice points are represented by null vectors and *lattice vectors* relating neighboring points are depicted in Fig. 3. Since each lattice vector is the normal for a plane through the lattice point, it is defined algebraically as half the vector difference between nearest neighbor points on each side of the plane. Therefore the set of all lattice vectors at a lattice point represents a set of planes intersecting at that point.

The translation symmetries of every 3D lattice are determined by a set of three lattice vectors a, b, c defining a *unit cell*. They determine a set of *primitive translations* generated by the versors $T_{\pm a}, T_{\pm b}, T_{\pm c}$, as explained in the preceding section. There is some arbitrariness in choosing the unit cell for a given lattice. We take advantage of that by choosing lattice vectors that also generate point symmetries of the lattice. We call these vectors *symmetry vectors*, as in suitable combinations they generate all the symmetries of the lattice. From the three symmetry vectors for each crystal we construct a minimal set of *symmetry versors* that generates the entire space group for the crystal. We have already discussed versors generating reflections, rotations, and translations. These can be combined to get new symmetry versors that generate glide reflections and screw displacements, as illustrated in Fig. 4. In this section we present a complete catalog of symmetry versors for all the space groups.

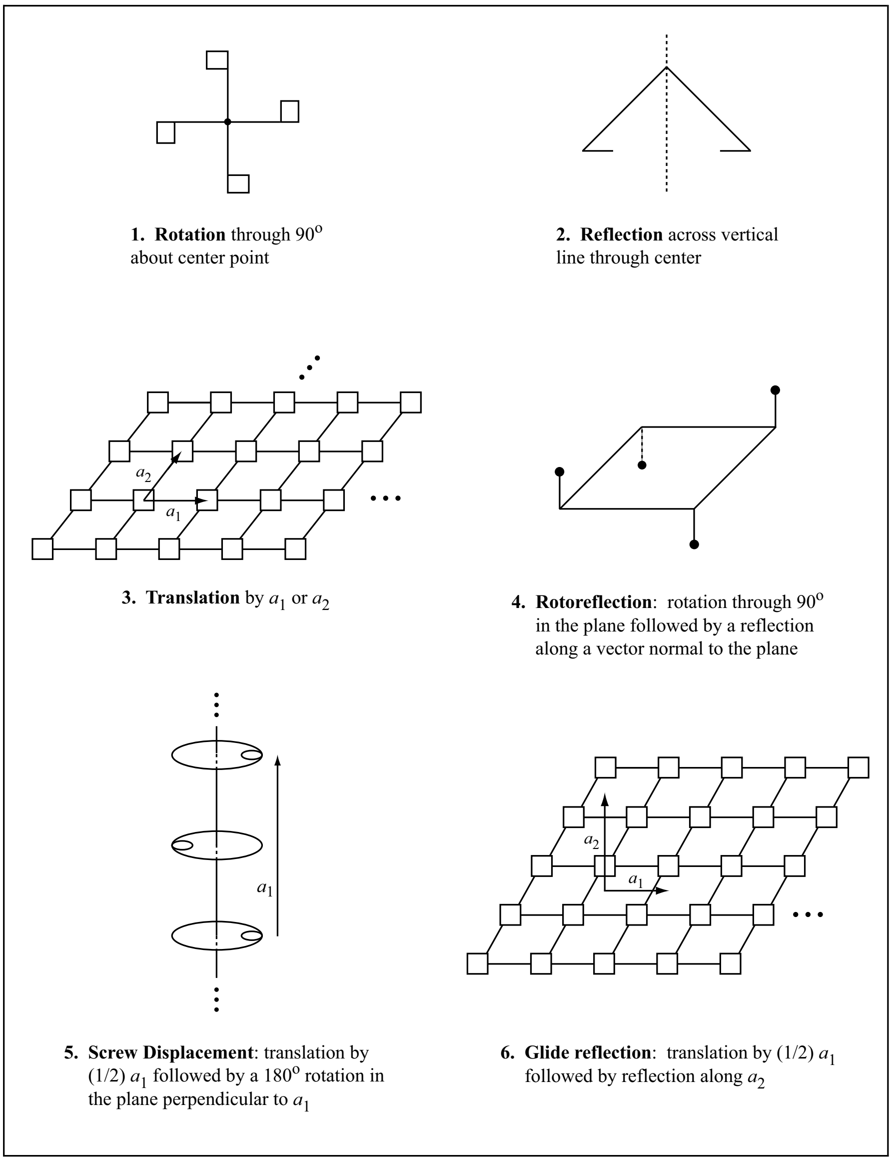

Fig. 4. Examples of the six types of symmetry transformations relevant to the crystallographic groups.

Standard symbols for the space groups [12, 15] do not take advantage of the important fact that each space group can be constructed from three symmetry vectors. For that reason we propose new symbols that enable one to write down generating versors for the groups directly. We have already introduced suitable symbols for the crystallographic point groups in Table 3. For the space groups we need to extend those symbols to describe how the point groups combine with translations. We aim to conform to the international symbol system [12, 15] as closely as possible. Accordingly, we adopt the standard classification of crystal lattices known as *Bravais lattices*, along with their subdivision into *crystal systems*, as shown in Fig. 5 for 2D lattices and Fig. 6 for 3D lattices. Crystal systems describe point

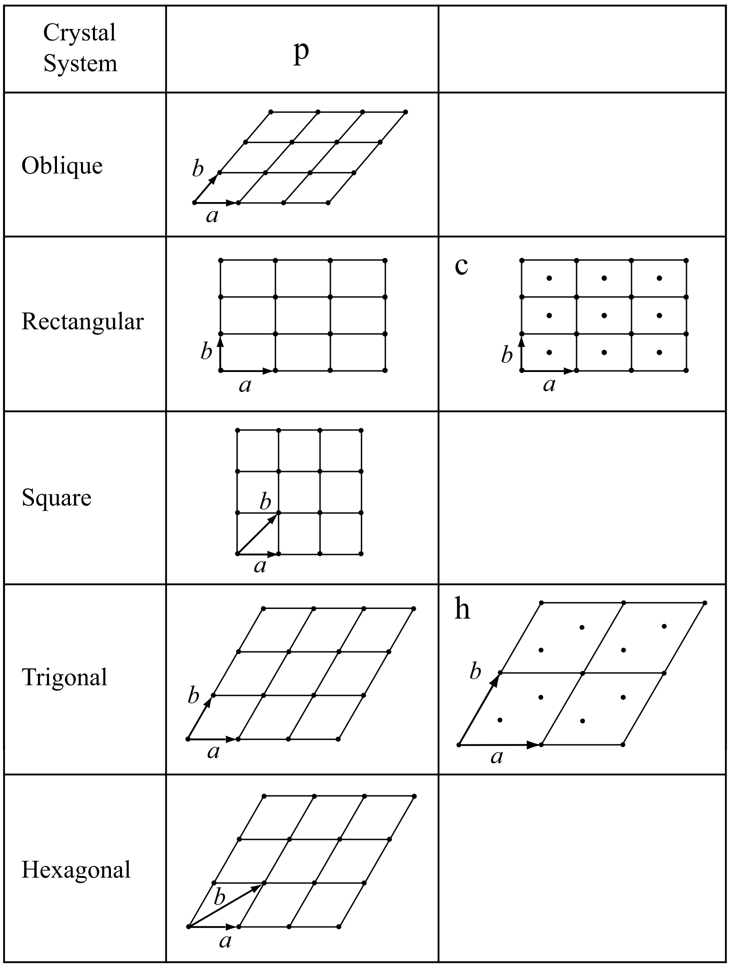

Fig. 5. The two-dimensional Bravais lattices and the associated symmetry vectors for each of the five crystal systems. For the trigonal system we have included the nonstandard "h" lattice.

symmetries, and each system is composed of the subgroups of a point group with maximal symmetry called the *holohedral group* of the system.

A complete list of symbols and versor generators for the 17 planar space groups and 230 space groups in 3D are given in Tables 4 and 5, except that we have omitted the primitive translations, because they are obvious, given the lattice type and the definitions of the symmetry vectors shown in Figs. 5 and 6. Note that we often suppress the distinction between space group elements and the versors that represent them. The remainder of this section is devoted to explaining the system of space group symbols and how the generators for each group can be constructed from them.

Each space group symbol designates a lattice type, point group, and joining constraints. The symbol for lattice type specifies the Bravais lattice and hence the nonprimitive translational symmetries in the space group. The point group symbols and their associated generators have already been explained and listed in Table 3. Most important is the fact that the point group part of a space group symbol indicates the angles between the symmetry vectors in the Bravais lattice. Lastly, we define a *joining constraint* to be the product of a

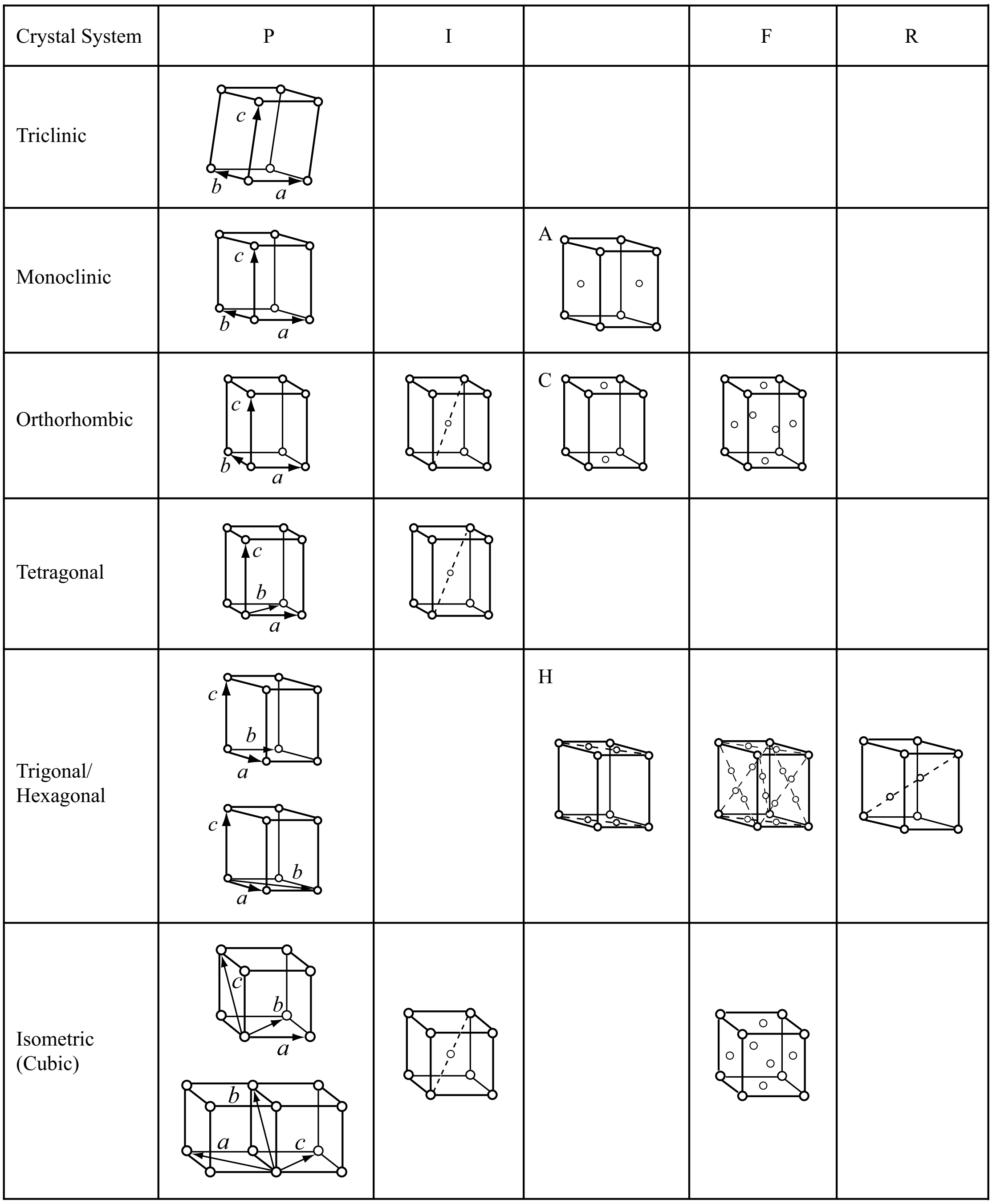

Fig. 6. The three-dimensional Bravais lattices and their symmetry vectors. Although not shown in the figure, the symmetry vectors for the nonprincipal lattices are the same as in the principal lattices. For the trigonal/hexagonal system we have introduced two new lattices labeled “H” and “F.”

	International Notation	Geometric Notation	Space Group Generators
	Oblique		
1	p1	$p\bar{1}$	
2	p2	$p\bar{2}$	$a \wedge b$
	Rectangular		
3	pm	p1	a
4	pg	p_g1	$aT_b^{1/2}$
5	cm	c1	a
6	pmm	p2	a, b
7	pmg	p_g2	$aT_b^{1/2}, b$
8	pgg	p_g2_g	$aT_b^{1/2}, bT_a^{1/2}$
9	cmm	c2	a, b
	Square		
10	p4	$p\bar{4}$	ab
11	p4m	p4	a, b
12	p4g	p_g4	$aT_{b-a}^{1/2}, b$
	Trigonal		
13	p3	$p\bar{3}$	ab
14	p3m1	p3	a, b
15	p31m	h3	a, b
	Hexagonal		
16	p6	$p\bar{6}$	ab
17	p6m	p6	a, b

Table 4. The 17 two-dimensional space groups and their generators. Pure translation generators are omitted but can be obtained from Fig. 5. The 13 symmorphic space groups are listed in bold font.

point group generator with a subprimitive translation (that is, some fraction of a primitive translation) to produce a new kind of irreducible generator. Our main task is therefore to describe the various joining constraints. Space groups without a joining constraint are called *symmorphic*. In such groups both the point group and the translation group are independent subgroups, so all the group elements are generated by direct products of translation and point group generators. For more details we examine the 2D and 3D space groups separately.

5.1. Planar Space Groups

Unit cells for the five Bravais lattices in 2D are depicted in Fig. 5. The unit cell of a *primitive*, or "p," lattice contains a single lattice point (at the cell vertex). The unit cell of a *centered*, or "c," lattice contains two points. Although the hexagonally centered, or "h," lattice has been largely neglected in the literature, we find that it has a natural place in the geometric algebra description of the space groups. For further discussion of the h lattice and its three-dimensional generalization, see Chapter 5 of [12].

There are 13 symmorphic space groups in 2D, identified by bold numbers in Table 4. Among these, all translations in the primitive lattices are generated by primitive generators, so only the point group generators are listed in Table 4. The centered lattices for groups c1 and c2 require the subprimitive generator $T_{a+b}^{1/2} = T_{(a+b)/2}$ for translations to the centered point. Lattices for the groups p3 and h3 are the same, but their unit cells are different. In the h lattice the versor $T_{a+b}^{1/3}$ generates subprimitive translations to two lattice points inside the cell.

One special feature of some point groups deserves mention. The bivector $a \wedge b$ is the directed area of a unit cell in the plane. It is also the versor generator of *inversion in the plane*, which is better regarded as a rotation by 180°. Indeed, it satisfies the constraint for a 2-fold rotation group:

$$(a \wedge b)^2 = -|a \wedge b|^2 \doteq -1, \tag{29}$$

which is a subgroup for the oblique space group p$\bar{2}$, listed as group #2 in Table 4. It is also a generator in other versor groups when $a \cdot b = 0$ so that $a \wedge b = ab$.

It should be noted that composition of a reflection with a primitive translation in the normal direction displaces the reflection line (or plane) by half a unit cell. This is demonstrated algebraically by

$$aT_a = T_a^{-1}a = T_a^{-1/2}aT_a^{1/2}, \tag{30}$$

where we have used the fact that a anticommutes with e in the translation versor defined in (26). The last expression in this equation exhibits the translation explicitly. This displaced reflection versor appears already in the group p1 #3 in Table 4.

The 4 remaining non-symmorphic space groups are constructed by replacing reflections in symmorphic groups by *glide reflections*, which are reflections in a mirror line (or plane in 3D) composed with a subprimitive translation parallel to that line (or plane). Algebraically, a glide generator is constructed by multiplying the reflection normal by a subprimitive translation versor. In Table 4, the presence of this particular type of "joining constraint" is indicated by inserting a "g" in the group symbol. As the point group symbol refers to two reflection generators a, b, we indicate replacement of the reflection generator a by placing the g before that symbol and replacement of b by placing it after the symbol.

In the group p_g1, the glide versor is given by

$$G_b \equiv aT_{b/2} = T_{b/2}a. \tag{31}$$

The commutativity of reflection and translation in this expression follows from the fact that a anticommutes with both b and e in (26). It follows that $G_b^2 = a^2T_b \doteq T_b$, so G_b is a kind of square root of the primitive translation T_b. This is characteristic of all glide reflections.

The glide generator in the group p_g2 is also given by G_b. Depending on how we choose to arrange the lattice points, we must either (a) displace the remaining reflection generator to $bT_b/2 = T_{b/4}^{-1}bT_{b/4}$ (which is the convention in [12]) or (b) place the lattice points at the intersection of the two reflection planes. In (a) the product of these two group generators gives us the rotation group element, as explicitly expressed by $G_b(bT_{b/2}) = aT_{b/2}bT_{b/2} = ab$, and in (b) this rotation is displaced by $T_b^{1/4}$. To obtain the simplest expressions for the generators, we use the convention that the lattice points be located at the intersection of the two reflection planes. More will be said about this in the following sections.

In the space group p_g2_g the joining constraints are essentially the same, except that reflection b is changed into the glide reflection $bT_a^{1/2}$. In the remaining nonsymmorphic planar group p_g4, there is a glide reflection with generator $aT_{b-a}^{1/2}$, because in the square lattice the direction normal to a is given by $b - a$.

5.2. Space Groups in 3D

Unit cells for the 14 Bravais lattices in 3D are depicted in Fig. 6 and generated by three symmetry vectors a, b, c, as we have already explained. For both the trigonal/hexagonal and cubic systems there are two sets of possible symmetry vectors. The point group part of the space group symbol, which defines the angles between a, b, and c, determines which set of symmetry vectors is to be used. The point group rotation generators ab, bc, ca determine faces of the unit cell conventionally designated by C, A, B, respectively. We can interpret the face symbols as bivectors representing directed areas such as $C \equiv a \wedge b$ and likewise for the other faces. The directed volume of a unit cell is a trivector $I \equiv a \wedge b \wedge c$, also called the *cell pseudoscalar*. The pseudoscalar is the versor generator of *(space) inversion*, with the group property

$$I^2 = -|I|^2 \doteq -1, \tag{32}$$

and it is listed as the sole point group generator for the oblique space group P$\overline{22}$ in Table 5. It generates inversions in many other groups as well, as we see below.

As depicted in Fig. 6, there are several types of lattices, designated as *primitive* (P), *body-centered* (I), *single-face centered* (A, B or C), *face-centered* (F), *rhombohedral* (R), and *hexagonal* (H). Note that in the trigonal/hexagonal system we have included both a hexagonal and face-centered lattice. As we mentioned in the previous subsection, the hexagonal lattice is well-established though largely neglected in current discussions of the space groups. However, it appears naturally in our GA formulation for which several space groups require that we define symmetry vectors along the edges of an H lattice. Moreover, we are led to introduce a face-centered lattice in the trigonal/hexagonal system, which is obtained from a traditional R lattice along with symmetry vectors defined as in the H lattice. These lattice symbols along with the point group symbols are all we need to define the 73 symmorphic space groups in 3D (indicated by bold group numbers in Table 5).

Lattices in the *Monoclinic System* have unit cells with one symmetry vector c orthogonal to the others. (Note: The International Tables [12] choose b rather than c, which accounts for some differences in our group symbols.) It follows that the cell pseudoscalar factors into $I = Cc$, where $C = a \wedge b$ is the generator of rotations in group #3, P$\bar{2}$. We can solve for $C \doteq Ic$, which expresses the rotation as a product of space inversion and a reflection. Enlarging the symmetry group to include the reflection $c \doteq CI$, we get group #10, P$\bar{2}$2. In this case any two of the three versors C, I, c can be chosen as generators of the point symmetries. From these two groups, we get groups #5 and #12 for A-centered lattices simply by adding the subprimitive $T_{(b+c)/2}$ to the set of generators.

Construction of the non-symmorphic 3D space groups proceeds by identifying joining constraints just as we did in the 2D case, except there are many more possibilities. There are two general classes of constraints joining subprimitive translations to point symmetries: *glide reflections* replacing reflections and *screw displacements* replacing rotations. Everything we said about glide reflections in 2D carries over to 3D, where the

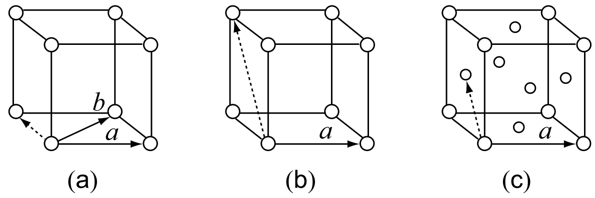

Fig. 7. Examples of different types of glide reflections. In each case the reflection is generated by the vector a and the translational component is along the dashed vector through one-half its length. (a) An axial b-glide reflection, (b) a diagonal glide, (c) a diamond glide.

glide lines automatically become glide planes. In 3D there are three types of glide: *axial glides*, *diagonal glides*, and *diamond glides*, as depicted in Fig. 7. To distinguish the different possibilities, in the group symbol we insert one of the five letters a, b, c; n; d. In an axial glide the translation is along one of the edges of the Bravais lattice. Although the symmetry vectors do not always lie on the edge of a Bravais lattice, we can nevertheless choose a unit cell that associates each symmetry vector with a lattice edge. Accordingly, we label axial glide reflections by the associated symmetry vector, which yields an a-glide, b-glide, or c-glide. For instance, in 3D space group #100 the a reflection is replaced by the b-glide reflection $aT_{a-b}^{1/2}$. The "n" designates a *diagonal* n-glide in which the translation is along a diagonal of any of the three cell faces or along the diagonal through the center of the cell. Finally, a *diamond* glide occurs only in "F" and "I" lattices, where the glide translation is half the distance to a lattice point in the middle of a face or the center of the cell. As in the 2D case, the reflection being replaced by a glide is indicated in the space group symbol by placing the glide letter adjacent to the symbol associated with the reflection. For example, in space groups #61, #62, and #63, the reflections being replaced are $\{a, b, c\}$, $\{a, c\}$, and $\{b\}$ respectively. Thus, to ascertain the generators for the space group $\mathrm{P}_n 22_a$ (#62), the first reflection changes into a diagonal glide with translational component $T_{b+c}^{1/2}$; the second reflection remains unchanged, and the third reflection changes to an a-glide with translational factor $T_a^{1/2}$. Hence, the non-translational generators are $aT_{b+c}^{1/2}, b$, and $cT_a^{1/2}$.

Rotations, represented in the space group symbol by numbers with overbars, can be converted into screw displacements. For a rotation represented by $\bar{m}$, the possible screw displacements are $\bar{m}_1, \bar{m}_2, \ldots, \bar{m}_{m-1}$. Fig. 8 shows the different screw displacements for each of the allowed rotations. From this figure one can construct the translational and rotational components of screw displacements. For example, in the space group $\mathrm{P}\bar{4}_1\bar{2}_1\bar{2}$ (space group #92), the basic generators are ab and bc. The first rotation is changed into the screw displacement $abT_c^{1/4}$. The second rotation is turned into the screw displacement $bcT_{2a-b}^{1/2}$, since the direction perpendicular to the bc plane is along $2a - b$. Finally, there are several instances in which the rotation axes for the generators ab and bc do not intersect. In these cases the rotation generator must also include a translational component. For instance, space groups #18 and #19 both have the basic generators $abT_c^{1/2}$ and $bcT_a^{1/2}$, but in space group #19 the two axes do not intersect. In fact, the bc rotation axis is displaced from the ab axis by the translation $T_b^{1/4}$. Therefore, in space group #19 the generators are $abT_c^{1/2}$ and $T_b^{-1/4}[bcT_a^{1/2}]T_b^{1/4}$. Similarly, in space groups #195 and #198, the generators are $\{ab, bc\}$ and $\{ab, T_{a+c}^{-1/4} bcT_{a+c}^{1/4}\}$, respectively.

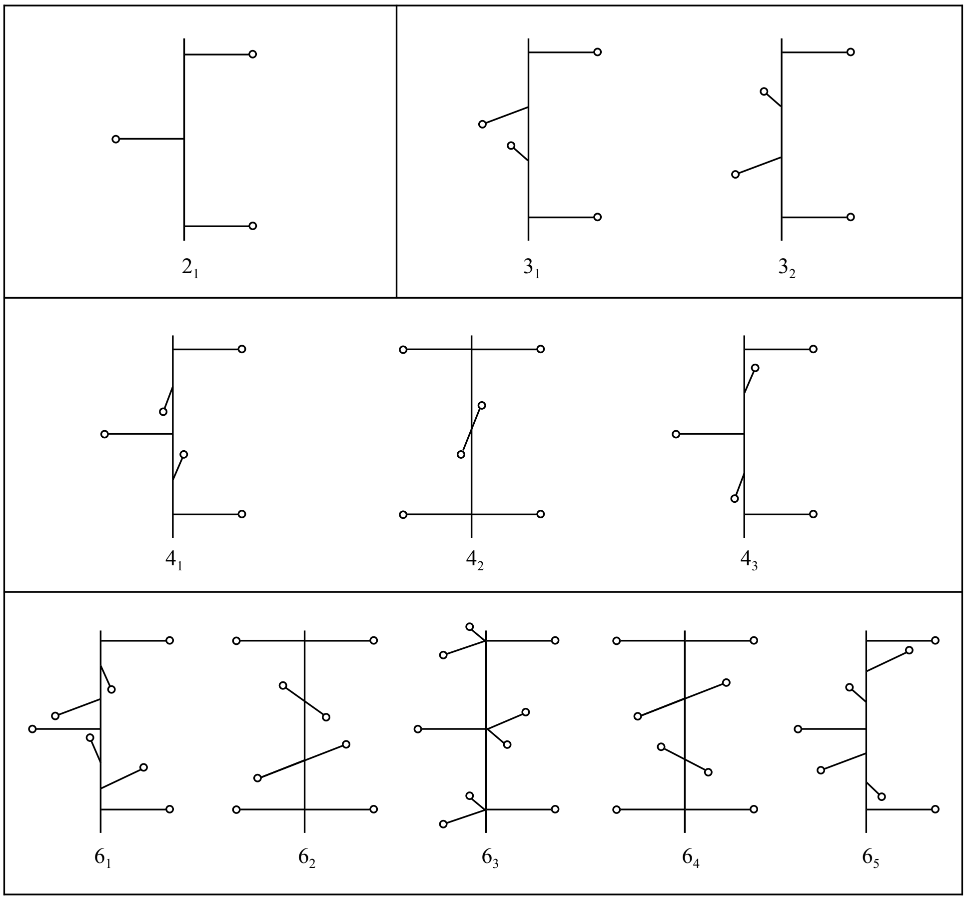

Fig. 8. Figures exhibiting the different types of screw displacement symmetries found in the 3D space groups. This figure is based on Fig. 2 in Chapter 8 of [13].

5.3. Alternate Presentations and Notations for the Space Groups

We are open to improvements in the space group symbols, though we are perfectly satisfied with the formulation of group structure in Conformal GA. For example, in group #61, the short Hermann-Maugin symbol Pbca is evidently simpler than our symbol $P_b 2_c 2_a$. Indeed, the latter uses five symbols to designate only three generators. The question, though, is whether the rotation structure designated by the 2's contributes to unambiguous identification of the group generators and/or the orderly classification of space groups. In fact, when compared to the full Hermann-Maugin symbol for this space group, $P2_1/b2_1/c2_1/a$, the GA symbol is more concise. Another nomenclature for the classification of the space groups is the Hall notation [16], which enables one to systematically write down the 4×4 Seitz matrices for the symmetry transformations directly from the group symbol. Comparison of the GA notation with this and other classification schemes will be an important future endeavor.

Our notation scheme is based on taking the three symmetry vectors and their properties as primary. Their lengths are lattice constants and the angles between them are determined by their multiplicative properties. The purpose of the notation, therefore, is to specify how these vectors combine to create generators for the various groups. We note, though, that there are often several alternative sets of generators, so the preferred choice depends on one's purposes. For example, in 3D space group #218 the generators we've listed are $aT^{1/4}_{2b-a+c}, bT^{1/4}_{2b-c-3a}$, and $cT^{1/4}_{2b-c+a}$. However, there is a simpler set of generators: $\{ab, bc, cT^{1/4}_{2b-c+a}\}$. Equivalence of the two sets is shown by

$$\begin{aligned} [bc][cT^{1/4}_{2b-c+a}][T_{-a}] &\doteq bT^{1/4}_{2b-c-3a} \\ [ab][bT^{1/4}_{2b-c-3a}][T^{1/2}_{a+c}] &\doteq aT^{1/4}_{2b-a+c}. \end{aligned} \tag{33}$$

We have chosen the former presentation because it conforms to the simple desiderata in our notational scheme: we construct new space groups by replacing the generators listed in Table 3 with glide reflections or screw displacements. This raises the question: Is there a notation scheme that unambiguously designates an optimal set of generators?

There is also much freedom in the choice of lattice points and unit cells. As we mentioned before, we have chosen lattice points that allow the most straightforward constructions of space group generators, and this occasionally differs from standard conventions in [12]. Other choices may be preferred, for example, to locate certain molecular clusters in a crystal at lattice points. Thus, applications of our GA formulation to practical problems of crystallography may call for different choices of both lattice points and space group presentations. However, we are confident that the formalism is flexible enough to accommodate any necessary changes.

6. Conclusions

Group theory provides a general mathematical framework for describing symmetries in the structure and properties of a physical system. In specific applications, however, other mathematical tools are needed to characterize group elements and invariants. This paper has introduced *conformal GA* as a new tool to characterize the crystallographic space groups. In explicating the simple versor representations of the classical space groups, we have de-emphasized the ambiguity in sign, though we have noted that the sign distinguishes geometric objects of opposite orientation. That point has not gone unnoticed in the literature. In particular, Shubnikov noticed that the sign can be used to associate a color with each reflection, which led to an extension of the space groups to a much larger class of dichromatic (Shubnikov) space groups [17]. Conformal GA has not yet been applied to a detailed treatment of the Shubnikov groups, though we expect the task to be fairly straightforward. Of course, there is much more to crystallography than the space groups, so there is much more to be done in applying Conformal GA to the subject.

Our treatment of the space groups illustrates the power of Conformal GA as a general formalism for molecular modeling. The approach is especially promising for modeling geometry of large biological molecules and dynamical systems with strong coupling between translational and rotational degrees of freedom [18]. Finally, we submit that Conformal GA will prove to be an important component of the general program to unify mathematical physics with geometric algebra and thus provide students with earlier access to advanced tools and topics in physics [3].

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	Internat. Notat.	Geom. Notat.	Space Group Generators		Internat. Notat.	Geom. Notat.	Space Group Generators
	Triclinic				Orthorhombic (cont.)		
1	P1	$\mathrm{P}\bar{1}$		**23**	I222	$\mathrm{I}\bar{2}\bar{2}\bar{2}$	ab, bc
2	$\mathrm{P}\bar{1}$	$\mathrm{P}\overline{22}$	$a \wedge b \wedge c$	24	$\mathrm{I}2_12_12_1$	$\mathrm{I}\bar{2}\bar{2}_1\bar{2}_1$	$ab, bcT_a^{1/2}$
	Monoclinic			**25**	Pmm2	P2	a, b
3	P2	$\mathrm{P}\bar{2}$	$a \wedge b$	26	$\mathrm{Pmc}2_1$	$\mathrm{P}2_c$	$a, bT_c^{1/2}$
4	$\mathrm{P}2_1$	$\mathrm{P}\bar{2}_1$	$(a \wedge b)T_c^{1/2}$	27	Pcc2	P_c2_c	$aT_c^{1/2}, bT_c^{1/2}$
5	C2	$\mathrm{A}\bar{2}$	$a \wedge b$	28	Pma2	$\mathrm{P}2_a$	$a, bT_a^{1/2}$
6	Pm	P1	c	29	$\mathrm{Pca}2_1$	P_c2_a	$aT_c^{1/2}, bT_a^{1/2}$
7	Pc	P_a1	$cT_a^{1/2}$	30	Pnc2	P_n2_c	$aT_{b+c}^{1/2}, bT_c^{1/2}$
8	Cm	A1	c	31	$\mathrm{Pmn}2_1$	$\mathrm{P}2_n$	$a, bT_{a+c}^{1/2}$
9	Cc	A_a1	$cT_a^{1/2}$	32	Pba2	P_b2_a	$aT_b^{1/2}, bT_a^{1/2}$
10	P2/m	$\mathrm{P}2\bar{2}$	$c, a \wedge b$	33	$\mathrm{Pna}2_1$	P_n2_a	$aT_{b+c}^{1/2}, bT_a^{1/2}$
11	$\mathrm{P}2_1/\mathrm{m}$	$\mathrm{P}2\bar{2}_1$	$c, (a \wedge b)T_c^{1/2}$	34	Pnn2	P_n2_n	$aT_{b+c}^{1/2}, bT_{a+c}^{1/2}$
12	C2/m	$\mathrm{A}2\bar{2}$	$c, a \wedge b$	**35**	Cmm2	C2	a, b
13	P2/c	$\mathrm{P}_a2\bar{2}$	$cT_a^{1/2}, a \wedge b$	36	$\mathrm{Cmc}2_1$	$\mathrm{C}2_c$	$a, bT_c^{1/2}$
14	$\mathrm{P}2_1/\mathrm{c}$	$\mathrm{P}_a2\bar{2}_1$	$cT_a^{1/2}, (a \wedge b)T_c^{1/2}$	37	Ccc2	C_c2_c	$aT_c^{1/2}, bT_c^{1/2}$
15	C2/c	$\mathrm{A}_a2\bar{2}$	$cT_a^{1/2}, a \wedge b$	**38**	Amm2	A2	a, b
	Orthorhombic			39	Aem2	A_b2	$aT_b^{1/2}, b$
16	P222	$\mathrm{P}\bar{2}\bar{2}\bar{2}$	ab, bc	40	Ama2	$\mathrm{A}2_a$	$a, bT_a^{1/2}$
17	$\mathrm{P}222_1$	$\mathrm{P}\bar{2}_1\bar{2}\bar{2}$	$abT_c^{1/2}, bc$	41	Aea2	A_b2_a	$aT_b^{1/2}, bT_a^{1/2}$
18	$\mathrm{P}2_12_12$	$\mathrm{P}\bar{2}_1\bar{2}_1\bar{2}$	$abT_c^{1/2}, bcT_a^{1/2}$	**42**	Fmm2	F2	a, b
19	$\mathrm{P}2_12_12_1$	$\mathrm{P}\bar{2}_1\bar{2}_1\bar{2}_1$	$abT_c^{1/2}, T_b^{-1/4}bcT_a^{1/2}T_b^{1/4}$	43	Fdd2	F_d2_d	$aT_{b+c}^{1/4}, bT_{a+c}^{1/4}$
20	$\mathrm{C}222_1$	$\mathrm{C}\bar{2}_1\bar{2}\bar{2}$	$abT_c^{1/2}, bc$	**44**	Imm2	I2	a, b
21	C222	$\mathrm{C}\bar{2}\bar{2}\bar{2}$	ab, bc	45	Iba2	I_b2_a	$aT_b^{1/2}, bT_a^{1/2}$
22	F222	$\mathrm{F}\bar{2}\bar{2}\bar{2}$	ab, bc	46	Ima2	$\mathrm{I}2_a$	$a, bT_a^{1/2}$

Table 5. The 230 three-dimensional space groups and their generators. Pure translation generators have been omitted but can be obtained from Fig. 6. Note that some space groups in the cubic system have the pure translation symmetry $T_{a+c}^{1/2}$ even for P lattices. The 73 symmorphic space groups are listed in bold font.

	International Notation	Geometric Notation	Space Group Generators		International Notation	Geometric Notation	Space Group Generators
	Orthorhombic (cont.)				Orthorhombic (cont.)		
47	Pmmm	P22	a, b, c	**71**	Immm	I22	a, b, c
48	Pnnn	P$_n$2$_n$2$_n$	$aT_{b+c}^{1/2}, bT_{a+c}^{1/2}, cT_{a+b}^{1/2}$	72	Ibam	I$_b$2$_a$2	$aT_b^{1/2}, bT_a^{1/2}, c$
49	Pccm	P$_c$2$_c$2	$aT_c^{1/2}, bT_c^{1/2}, c$	73	Ibca	I$_b$2$_c$2$_a$	$aT_b^{1/2}, bT_c^{1/2}, cT_a^{1/2}$
50	Pban	P$_b$2$_a$2$_n$	$aT_b^{1/2}, bT_a^{1/2}, cT_{a+b}^{1/2}$	74	Imma	I22$_a$	$a, b, cT_a^{1/2}$
51	Pmma	P22$_a$	$a, b, cT_a^{1/2}$		Tetragonal		
52	Pnna	P$_n$2$_n$2$_a$	$aT_{b+c}^{1/2}, bT_{a+c}^{1/2}, cT_a^{1/2}$	**75**	P4	P$\bar{4}$	ab
53	Pmna	P2$_n$2$_a$	$a, bT_{a+c}^{1/2}, cT_a^{1/2}$	76	P4$_1$	P$\bar{4}_1$	$abT_c^{1/4}$
54	Pcca	P$_c$2$_c$2$_a$	$aT_c^{1/2}, bT_c^{1/2}, cT_a^{1/2}$	77	P4$_2$	P$\bar{4}_2$	$abT_c^{1/2}$
55	Pbam	P$_b$2$_a$2	$aT_b^{1/2}, bT_a^{1/2}, c$	78	P4$_3$	P$\bar{4}_3$	$abT_c^{3/4}$
56	Pccn	P$_c$2$_c$2$_n$	$aT_c^{1/2}, bT_c^{1/2}, cT_{a+b}^{1/2}$	**79**	I4	I$\bar{4}$	ab
57	Pbcm	P$_b$2$_c$2	$aT_b^{1/2}, bT_c^{1/2}, c$	80	I4$_1$	I$\bar{4}_1$	$abT_c^{1/4}$
58	Pnnm	P$_n$2$_n$2	$aT_{b+c}^{1/2}, bT_{a+c}^{1/2}, c$	**81**	P$\bar{4}$	P$\overline{42}$	bac
59	Pmmn	P22$_n$	$a, b, cT_{a+b}^{1/2}$	**82**	I$\bar{4}$	I$\overline{42}$	bac
60	Pbcn	P$_b$2$_c$2$_n$	$aT_b^{1/2}, bT_c^{1/2}, cT_{a+b}^{1/2}$	**83**	P4/m	P$\bar{4}$2	ab, c
61	Pbca	P$_b$2$_c$2$_a$	$aT_b^{1/2}, bT_c^{1/2}, cT_a^{1/2}$	84	P4$_2$/m	P$\bar{4}_2$2	$abT_c^{1/2}, c$
62	Pnma	P$_n$22$_a$	$aT_{b+c}^{1/2}, b, cT_a^{1/2}$	85	P4/n	P$\bar{4}_n$2	$ab, cT_b^{1/2}$
63	Cmcm	C2$_c$2	$a, bT_c^{1/2}, c$	86	P4$_2$/n	P$\bar{4}_{2n}$2	$abT_c^{1/2}, cT_b^{1/2}$
64	Cmce	C2$_c$2$_a$	$a, bT_c^{1/2}, cT_a^{1/2}$	**87**	I4/m	I$\bar{4}$2	ab, c
65	Cmmm	C22	a, b, c	88	I4$_1$/a	I$\bar{4}_{1a}$2	$abT_c^{1/4}, cT_a^{1/2}$
66	Cccm	C$_c$2$_c$2	$aT_c^{1/2}, bT_c^{1/2}, c$	**89**	P422	P$\bar{4}\bar{2}\bar{2}$	ab, bc
67	Cmme	C22$_a$	$a, b, cT_a^{1/2}$	90	P42$_1$2	P$\bar{4}\bar{2}_1\bar{2}$	$ab, bcT_{2a-b}^{1/2}$
68	Ccce	C$_c$2$_c$2$_a$	$aT_c^{1/2}, bT_c^{1/2}, cT_a^{1/2}$	91	P4$_1$22	P$\bar{4}_1\bar{2}\bar{2}$	$abT_c^{1/4}, bc$
69	Fmmm	F22	a, b, c	92	P4$_1$2$_1$2	P$\bar{4}_1\bar{2}_1\bar{2}$	$abT_c^{1/4}, bcT_{2a-b}^{1/2}$
70	Fddd	F$_d$2$_d$2$_d$	$aT_{b+c}^{1/4}, bT_{a+c}^{1/4}, cT_{a+b}^{1/4}$	93	P4$_2$22	P$\bar{4}_2\bar{2}\bar{2}$	$abT_c^{1/2}, bc$

	Internat. Notat.	Geom. Notat.	Space Group Generators		Internat. Notat.	Geom. Notat.	Space Group Generators
Tetragonal (cont.)				Tetragonal (cont.)			
94	$P4_22_12$	$P\bar{4}_2\bar{2}_1\bar{2}$	$abT_c^{1/2}, bcT_{2a-b}^{1/2}$	118	$P\bar{4}n2$	$P_n4\bar{2}$	$aT_{a-b+c}^{1/2}, bc$
95	$P4_322$	$P\bar{4}_3\bar{2}\bar{2}$	$abT_c^{3/4}, bc$	**119**	$I\bar{4}m2$	$I4\bar{2}$	a, bc
96	$P4_32_12$	$P\bar{4}_3\bar{2}_1\bar{2}$	$abT_c^{3/4}, bcT_{2a-b}^{1/2}$	120	$I\bar{4}c2$	$I_c4\bar{2}$	$aT_c^{1/2}, bc$
97	I422	$I\bar{4}\bar{2}\bar{2}$	ab, bc	**121**	$I\bar{4}2m$	$I\bar{2}4$	ac, b
98	$I4_122$	$I\bar{4}_1\bar{2}\bar{2}$	$abT_c^{1/4}, bc$	122	$I\bar{4}2d$	$I\bar{2}_d4$	$ac, bT_{2a-b+c}^{1/4}$
99	P4mm	P4	a, b	**123**	P4/mmm	P42	a, b, c
100	P4bm	P_b4	$aT_{a-b}^{1/2}, b$	124	P4/mcc	P_c4_c2	$aT_c^{1/2}, bT_c^{1/2}, c$
101	$P4_2cm$	P_c4	$aT_c^{1/2}, b$	125	P4/nbm	P_b42_n	$aT_{a-b}^{1/2}, b, cT_b^{1/2}$
102	$P4_2nm$	P_n4	$aT_{a-b+c}^{1/2}, b$	126	P4/nnc	$P_n4_c2_n$	$aT_{a-b+c}^{1/2}, bT_c^{1/2}, cT_b^{1/2}$
103	P4cc	P_c4_c	$aT_c^{1/2}, bT_c^{1/2}$	127	P4/mbm	P_b42	$aT_{a-b}^{1/2}, b, c$
104	P4nc	P_n4_c	$aT_{a-b+c}^{1/2}, bT_c^{1/2}$	128	P4/mnc	P_n4_c2	$aT_{a-b+c}^{1/2}, bT_c^{1/2}, c$
105	$P4_2mc$	$P4_c$	$a, bT_c^{1/2}$	129	P4/nmm	$P42_n$	$a, b, cT_b^{1/2}$
106	$P4_2bc$	P_b4_c	$aT_{a-b}^{1/2}, bT_c^{1/2}$	130	P4/ncc	$P_c4_c2_n$	$aT_c^{1/2}, bT_c^{1/2}, cT_b^{1/2}$
107	I4mm	I4	a, b	131	$P4_2/mmc$	$P4_c2$	$a, bT_c^{1/2}, c$
108	I4cm	I_c4	$aT_c^{1/2}, b$	132	$P4_2/mcm$	P_c42	$aT_c^{1/2}, b, c$
109	$I4_1md$	$I4_d$	$a, bT_{2a-b+c}^{1/4}$	133	$P4_2/nbc$	$P_b4_c2_n$	$aT_{a-b}^{1/2}, bT_c^{1/2}, cT_b^{1/2}$
110	$I4_1cd$	I_c4_d	$aT_c^{1/2}, bT_{2a-b+c}^{1/4}$	134	$P4_2/nnm$	P_n42_n	$aT_{a-b+c}^{1/2}, b, cT_b^{1/2}$
111	$P\bar{4}2m$	$P\bar{2}4$	ac, b	135	$P4_2/mbc$	P_b4_c2	$aT_{a-b}^{1/2}, bT_c^{1/2}, c$
112	$P\bar{4}2c$	$P\bar{2}_c4$	$ac, bT_c^{1/2}$	136	$P4_2/mnm$	P_n42	$aT_{a-b+c}^{1/2}, b, c$
113	$P\bar{4}2_1m$	$P\bar{2}_14$	$acT_{a-b}^{1/2}, b$	137	$P4_2/nmc$	$P4_c2_n$	$a, bT_c^{1/2}, cT_b^{1/2}$
114	$P\bar{4}2_1c$	$P\bar{2}_{1c}4$	$acT_{a-b}^{1/2}, bT_c^{1/2}$	138	$P4_2/ncm$	P_c42_n	$aT_c^{1/2}, b, cT_b^{1/2}$
115	$P\bar{4}m2$	$P4\bar{2}$	a, bc	**139**	I4/mmm	I42	a, b, c
116	$P\bar{4}c2$	$P_c4\bar{2}$	$aT_c^{1/2}, bc$	140	I4/mcm	I_c42	$aT_c^{1/2}, b, c$
117	$P\bar{4}b2$	$P_b4\bar{2}$	$aT_{a-b}^{1/2}, bc$	141	$I4_1/amd$	$I4_d2_a$	$a, bT_{2a-b+c}^{1/4}, cT_a^{1/2}$

	Internat. Notat.	Geom. Notat.	Space Group Generators		Internat. Notat.	Geom. Notat.	Space Group Generators
	Tetragonal (cont.)				Trigonal (cont.)		
142	$I4_1/acd$	$I_c4_d2_a$	$aT_c^{1/2}, bT_{2a-b+c}^{1/4}, cT_a^{1/2}$	165	$P\bar{3}c1$	$P_c6\bar{2}$	$aT_c^{1/2}, bc$
	Trigonal			**166**	$R\bar{3}m$	$R6\bar{2}$	a, bc
143	$P3$	$P\bar{3}$	ab	167	$R\bar{3}c$	$R_c6\bar{2}$	$aT_c^{1/2}, bc$
144	$P3_1$	$P\bar{3}_1$	$abT_c^{1/3}$		Hexagonal		
145	$P3_2$	$P\bar{3}_2$	$abT_c^{2/3}$	**168**	$P6$	$P\bar{6}$	ab
146	$R3$	$R\bar{3}$	ab	169	$P6_1$	$P\bar{6}_1$	$abT_c^{1/6}$
147	$P\bar{3}$	$P\overline{6}\overline{2}$	bac	170	$P6_5$	$P\bar{6}_5$	$abT_c^{5/6}$
148	$R\bar{3}$	$R\overline{6}\overline{2}$	bac	171	$P6_2$	$P\bar{6}_2$	$abT_c^{1/3}$
149	$P312$	$P\bar{3}\bar{2}$	ab, bc	172	$P6_4$	$P\bar{6}_4$	$abT_c^{2/3}$
150	$P321$	$H\bar{3}\bar{2}$	ab, bc	173	$P6_3$	$P\bar{6}_3$	$abT_c^{1/2}$
151	$P3_112$	$P\bar{3}_1\bar{2}$	$abT_c^{1/3}, bc$	**174**	$P\bar{6}$	$P\bar{3}2$	ab, c
152	$P3_121$	$H\bar{3}_1\bar{2}$	$abT_c^{1/3}, bc$	**175**	$P6/m$	$P\bar{6}2$	ab, c
153	$P3_212$	$P\bar{3}_2\bar{2}$	$abT_c^{2/3}, bc$	176	$P6_3/m$	$P\bar{6}_32$	$abT_c^{1/2}, c$
154	$P3_221$	$H\bar{3}_2\bar{2}$	$abT_c^{2/3}, bc$	**177**	$P622$	$P\bar{6}\bar{2}$	ab, bc
155	$R32$	$F\bar{3}\bar{2}$	ab, bc	178	$P6_122$	$P\bar{6}_1\bar{2}$	$abT_c^{1/6}, bc$
156	$P3m1$	$P3$	a, b	179	$P6_522$	$P\bar{6}_5\bar{2}$	$abT_c^{5/6}, bc$
157	$P31m$	$H3$	a, b	180	$P6_222$	$P\bar{6}_2\bar{2}$	$abT_c^{1/3}, bc$
158	$P3c1$	P_c3_c	$aT_c^{1/2}, bT_c^{1/2}$	181	$P6_422$	$P\bar{6}_4\bar{2}$	$abT_c^{2/3}, bc$
159	$P31c$	H_c3_c	$aT_c^{1/2}, bT_c^{1/2}$	182	$P6_322$	$P\bar{6}_3\bar{2}$	$abT_c^{1/2}, bc$
160	$R3m$	$R3$	a, b	**183**	$P6mm$	$P6$	a, b
161	$R3c$	R_c3_c	$aT_c^{1/2}, bT_c^{1/2}$	184	$P6cc$	P_c6_c	$aT_c^{1/2}, bT_c^{1/2}$
162	$P\bar{3}1m$	$P\bar{2}6$	ac, b	185	$P6_3cm$	P_c6	$aT_c^{1/2}, b$
163	$P\bar{3}1c$	$P\bar{2}_c6$	$ac, bT_c^{1/2}$	186	$P6_3mc$	$P6_c$	$a, bT_c^{1/2}$
164	$P\bar{3}m1$	$P6\bar{2}$	a, bc	**187**	$P\bar{6}m2$	$P32$	a, b, c

	Internat. Notat.	Geom. Notat.	Space Group Generators		Internat. Notat.	Geom. Notat.	Space Group Generators
	Hexagonal (cont.)				Cubic (cont.)		
188	$P\bar{6}c2$	P_c3_c2	$aT_c^{1/2}, bT_c^{1/2}, c$	**209**	F432	$F\bar{4}\bar{3}\bar{2}$	ab, bc
189	$P\bar{6}2m$	H32	a, b, c	210	$F4_132$	$F\bar{4}_1\bar{3}\bar{2}$	$T_{a-b}^{-3/4}abT_{a-b+c}^{1/4}T_{a-b}^{3/4}, bc$
190	$P\bar{6}2c$	H_c3_c2	$aT_c^{1/2}, bT_c^{1/2}, c$	**211**	I432	$I\bar{4}\bar{3}\bar{2}$	ab, bc
191	P6/mmm	P62	a, b, c	212	$P4_332$	$P\bar{4}_3\bar{3}\bar{2}$	$T_{a-b}^{-1/4}abT_{a-b+c}^{3/4}T_{a-b}^{1/4}, bc$
192	P6/mcc	P_c6_c2	$aT_c^{1/2}, bT_c^{1/2}, c$	213	$P4_132$	$P\bar{4}_1\bar{3}\bar{2}$	$T_{a-b}^{-3/4}abT_{a-b+c}^{1/4}T_{a-b}^{3/4}, bc$
193	$P6_3$/mcm	P_c62	$aT_c^{1/2}, b, c$	214	$I4_132$	$I\bar{4}_1\bar{3}\bar{2}$	$T_{a-b}^{-3/4}abT_{a-b+c}^{1/4}T_{a-b}^{3/4}, bc$
194	$P6_3$/mmc	$P6_c2$	$a, bT_c^{1/2}, c$	**215**	$P\bar{4}3m$	P33	a, b, c
	Cubic			**216**	$F\bar{4}3m$	F33	a, b, c
195	P23	$P\bar{3}\bar{3}\bar{2}$	ab, bc	**217**	$I\bar{4}3m$	I33	a, b, c
196	F23	$F\bar{3}\bar{3}\bar{2}$	ab, bc	218	$P\bar{4}3n$	$P_n3_n3_n$	$aT_{2b-a+c}^{1/4}, bT_{2b-c-3a}^{1/4}, cT_{2b-c+a}^{1/4}$
197	I23	$I\bar{3}\bar{3}\bar{2}$	ab, bc	219	$F\bar{4}3c$	$F_c3_c3_a$	$aT_c^{1/2}, bT_{c-a}^{1/2}, cT_a^{1/2}$
198	$P2_13$	$P\bar{3}\bar{3}\bar{2}_1$	$ab, T_{a+c}^{-1/4}bcT_{a+c}^{1/4}$	220	$I\bar{4}3d$	$I_d3_d3_d$	$aT_{2b-a+c}^{1/8}, bT_{2b-c-3a}^{1/8}, cT_{2b-c+a}^{1/8}$
199	$I2_13$	$I\bar{3}\bar{3}\bar{2}_1$	$ab, T_{a+c}^{-1/4}bcT_{a+c}^{1/4}$	**221**	$Pm\bar{3}m$	P43	a, b, c
200	$Pm\bar{3}$	$P4\bar{3}$	a, bc	222	$Pn\bar{3}n$	$P_n4_n3_n$	$aT_c^{1/2}, bT_{c-a}^{1/2}, cT_{3a-2b+c}^{1/2}$
201	$Pn\bar{3}$	$P_n4\bar{3}$	$aT_c^{1/2}, bc$	223	$Pm\bar{3}n$	$P4_n3_n$	$a, bT_{c-a}^{1/2}, cT_{3a-2b+c}^{1/2}$
202	$Fm\bar{3}$	$F4\bar{3}$	a, bc	224	$Pn\bar{3}m$	P_n43	$aT_c^{1/2}, b, c$
203	$Fd\bar{3}$	$F_d4\bar{3}$	$aT_c^{1/4}, bc$	**225**	$Fm\bar{3}m$	F43	a, b, c
204	$Im\bar{3}$	$I4\bar{3}$	a, bc	226	$Fm\bar{3}c$	$F4_c3_a$	$a, bT_{a-b+c}^{1/2}, cT_a^{1/2}$
205	$Pa\bar{3}$	$P_b4\bar{3}$	$aT_{a-b}^{1/2}, bc$	227	$Fd\bar{3}m$	F_d4_n3	$aT_c^{1/4}, bT_{c-a}^{1/2}, c$
206	$Ia\bar{3}$	$I_b4\bar{3}$	$aT_{a-b}^{1/2}, bc$	228	$Fd\bar{3}c$	$F_d4_c3_a$	$aT_c^{1/4}, bT_{a-b+c}^{1/2}, cT_a^{1/2}$
207	P432	$P\bar{4}\bar{3}\bar{2}$	ab, bc	**229**	$Im\bar{3}m$	I43	a, b, c
208	$P4_232$	$P\bar{4}_2\bar{3}\bar{2}$	$T_a^{-1/2}abT_{a-b+c}^{1/2}T_a^{1/2}, bc$	230	$Ia\bar{3}d$	$I_b4_d3_d$	$aT_{a-b}^{1/2}, bT_{c-a}^{1/4}, cT_{3a-2b+c}^{1/4}$