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A derivation of the 32 crystallographic point groups using elementary group theory

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Abstract

A rigorous derivation of the 32 crystallographic point groups is presented. The derivation is designed for scientists who wish to gain an appreciation of the group theoretical derivation but who do not wish to master the large number of specialized topics used in other rigorous group theoretical derivations.

Introduction

This paper has two objectives. The first is the very specific goal of giving a complete and rigorous derivation of the 32 crystallographic point groups with emphasis placed on making this paper as self-contained as possible. The second is the more general objective of presenting several concepts of modern mathematics and their applicability to the study of crystallography. Throughout the paper we have attempted to present as much of the mathematical theory as possible, without resorting to long digressions, so that the reader with only a modest amount of mathematical knowledge will be able to appreciate the derivation. Those facts that are used but not proven in this paper will be clearly identified and references will be given to sources where the appropriate discussions can be found.

Crystal symmetry was studied during the nineteenth century largely from a geometrical viewpoint. A comprehensive outline of the more important contributions to this subject by such men as Hessel, Bravais, Möbius, Gadolin, Curie, Federov, Minnigerode, Schoenflies, and Miers is presented by Swartz (1909). It appears that Minnigerode (1884), Schoenflies (1891), and Weber (1896) were the first to recast the problem of classifying crystal symmetry in terms of group theory. Recent treatments make extensive use of specialized topics in group theory in the derivation of the crystallographic point groups (see for example Seitz, 1934; Zachariasen, 1945; Burckhardt, 1947; Zassenhaus, 1949; Lomont, 1959; Weyl, 1952; McWeeny, 1963; Altmann, 1963; Yale, 1968; Benson and Grove, 1971; Janssen, 1973; Coxeter, 1973; and Senechal, 1976). In addition, several workers (for example, Donnay, 1942, 1967; Buerger, 1963) have appealed to a number of interesting algorithms based on various geometric and heuristic arguments to obtain the 32 crystallographic point groups. In this paper we present a rigorous derivation of the 32 crystallographic point groups that uses only the most elementary notions of group theory while still taking advantage of the power of the theory of groups.

The derivation given here was inspired by the discussions given in Klein (1884), Weber (1896), Zassenhaus (1949), and Weyl (1952). The mathematical approach used in their discussions is a blend of group theory and the theory of the equivalence relation. Each of these mathematical concepts is described herein and is used in the ways suggested by these authors. However we depart from their approach in the determination of the interaxial angles. While they appeal to a study of Platonic solids, we continue with the theory of groups and equivalence relations in our determination of these angles.

In the first part of the paper we discuss the definition and properties of point isometries and show that every point isometry is either a proper or an improper rotation. If a rotation leaves a lattice invariant, then it is shown that its turn angle must be one of the eight following possibilities: 0°, ±60°, ±90°, ±120°, 180°. The method for composing two point isometries is discussed. The properties discovered about this composition motivate the definition of an abstract group, which is then stated. We then show that the set of all point isometries that leaves a given lattice invariant forms a finite group. These are the crystallographic point groups. In the second part, the proper crystallographic groups are discussed. The cyclic monaxial crystallographic groups are treated first. Then the notion of an equivalence relation and equivalence classes are presented in conjunction with a group

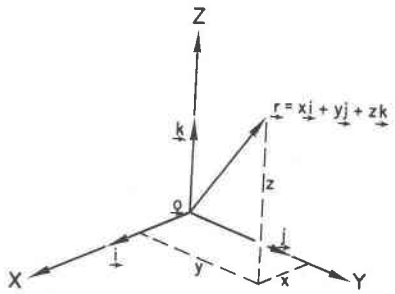

FIG 1. Right-handed cartesian coordinate system with unit vectors $\vec{i},\vec{j},\vec{k}$ directed along the coordinate axes X, Y, and Z, respectively, with the vector $\vec{r}$ expressed as a linear combination of $\vec{i}$, $\vec{j}$ and $\vec{k}$.

theoretical development of the basic ideas leading to the derivation of all the proper polyaxial crystallographic groups together with their interaxial angles. In the final part of the paper, the improper crystallographic groups are constructed from the proper crystallographic groups.

Discussion of basic concepts

Three dimensional space

Our discussion of the 32 crystallographic point groups will be conducted within the framework of real three-dimensional space, $\mathbf{R}^3$, where $\mathbf{R}$ designates the set of all real numbers. The elements of $\mathbf{R}^3$ can be described geometrically by placing three unit vectors, $\vec{i}$, $\vec{j}$ and $\vec{k}$ along three mutually perpendicular axes X, Y, and Z which form a right-handed cartesian coordinate system as in Figure 1. Accordingly, the vectors $\vec{i},\vec{j},\vec{k}$ form a basis for $\mathbf{R}^3$ such that $\mathbf{R}^3$ may be viewed as simply the collection of all linear combinations of the form $\vec{r} = x\vec{i} + y\vec{j} + z\vec{k}$ where x, y, z are elements of the set $\mathbf{R}$ (symbolized $x,y,z \in \mathbf{R}$). Note that x, y, and z are the X,Y and Z components of $\vec{r}$. Stated more concisely, $\mathbf{R}^3 = \{x\vec{i} + y\vec{j} + z\vec{k} \mid x,y,z \in \mathbf{R}\}$ which is read "$\mathbf{R}^3$ is the set of all vectors $x\vec{i} + y\vec{j} + z\vec{k}$ such that x,y,z are elements of the set $\mathbf{R}$." It is important to observe that each vector in $\mathbf{R}^3$ may be expressed in one and only one way as a linear combination of $\{\vec{i},\vec{j},\vec{k}\}$. We call the vector $\vec{O} = 0\vec{i} + 0\vec{j} + 0\vec{k}$ the origin of $\mathbf{R}^3$ and also use $\vec{O}$ to denote the point at the origin. In general, unless otherwise stated, we will not distinguish between a vector and its end-point. If $\vec{r} = x\vec{i} + y\vec{j} + z\vec{k}$ is some element of $\mathbf{R}^3$, then its magnitude or length, $\|\vec{r}\|$, is defined to be

$$\|\vec{r}\| = \sqrt{x^2 + y^2 + z^2}.$$

Point isometries

In our study of point groups we are interested in a special kind of transformation known as a point isometry. The mapping Φ from $\mathbf{R}^3$ onto $\mathbf{R}^3$ is a *point isometry* if and only if it satisfies the following four properties:

(1) Given any element $\vec{r} \in \mathbf{R}^3$, its image $\Phi(\vec{r})$ is a uniquely determined element of $\mathbf{R}^3$. (This means that Φ is a mapping from $\mathbf{R}^3$ to $\mathbf{R}^3$.)*

(2) Given any element $\vec{r} \in \mathbf{R}^3$, there exists an element $\vec{s} \in \mathbf{R}^3$ such that $\Phi(\vec{s}) = \vec{r}$. (This means that Φ is a mapping from $\mathbf{R}^3$ *onto* $\mathbf{R}^3$.)

(3) The magnitude of $\vec{r}$ is equal to the magnitude of the image of $\vec{r}$ under Φ for all $\vec{r} \in \mathbf{R}^3$, *i.e.*, $\|\vec{r}\| = \|\Phi(\vec{r})\|$. (This means that Φ preserves magnitudes and hence angles, sizes, and shapes.)

(4) Given any two elements $\vec{r}, \vec{s} \in \mathbf{R}^3$, $\Phi(\vec{r} + \vec{s}) = \Phi(\vec{r}) + \Phi(\vec{s})$ and given any real number x, $\Phi(x\vec{r}) = x\Phi(\vec{r})$. In particular, if $\vec{r} = x\vec{i} + y\vec{j} + z\vec{k}$, then $\Phi(\vec{r}) = x\Phi(\vec{i}) + y\Phi(\vec{j}) + z\Phi(\vec{k})$. (This means that Φ is a *linear tranformation* and that $\Phi(\vec{r})$ is completely determined by $\Phi(\vec{i})$, $\Phi(\vec{j})$ and $\Phi(\vec{k})$.)

A consequence of these properties is that Φ is a *one-to-one* mapping. That is, if $\vec{r}$ and $\vec{s}$ are in $\mathbf{R}^3$ such that $\vec{r} \neq \vec{s}$, then $\Phi(\vec{r}) \neq \Phi(\vec{s})$. Equivalently, if $\Phi(\vec{r}) = \Phi(\vec{s})$ for some $\vec{r},\vec{s} \in \mathbf{R}^3$, then $\vec{r}$ must equal $\vec{s}$. A consequence of property (4) is that $\Phi(\vec{O}) = \Phi(0\vec{i} + 0\vec{j} + 0\vec{k}) = 0\Phi(\vec{i}) + 0\Phi(\vec{j}) + 0\Phi(\vec{k}) = \vec{O}$. Hence the origin $\vec{O}$ of $\mathbf{R}^3$ is fixed under Φ, *i.e.*, $\Phi(\vec{O}) = \vec{O}$. (The word "point" in point isometry and point group alludes to the property that some point, in this case the origin, is left fixed—that is, unchanged in position—by Φ.)

If Θ and Φ are two point isometries, then we say that they are equal—that is $\Theta = \Phi$—if $\Theta(\vec{r}) = \Phi(\vec{r})$ for all $\vec{r} \in \mathbf{R}^3$. Hence in view of (4), two point isometries Θ and Φ are equal if and only if $\Theta(\vec{i}) = \Phi(\vec{i})$, $\Theta(\vec{j}) = \Phi(\vec{j})$ and $\Theta(\vec{k}) = \Phi(\vec{k})$. A trivial but important example of a point isometry is the identity mapping I on $\mathbf{R}^3$ defined by $I(\vec{r}) = \vec{r}$ for all $\vec{r} \in \mathbf{R}^3$. In the case of the identity mapping, magnitudes are preserved since under I each vector in $\mathbf{R}^3$ is mapped onto itself. Another example of a point isometry is a rotation. For our purposes a rotation will mean a turning of space about a line, called the rotation axis, that goes through $\vec{O}$ and has a positive direction

* In general, a *mapping* α of a set $\mathbf{A}$ into a set $\mathbf{B}$ is a rule which assigns to each element in $\mathbf{A}$ a unique element in $\mathbf{B}$. In this paper, $\mathbf{R}^3$ plays the role of both $\mathbf{A}$ and $\mathbf{B}$, that is, the mapping we will be using will map $\mathbf{R}^3$ into $\mathbf{R}^3$.

defined on it. Let **P** denote such a rotation and let ℓ denote its rotation axis. Then a turn angle ρ of **P** is an angle measuring the action of **P** on a plane perpendicular to ℓ. The turn angle is considered to be positive if the action of the rotation is measured in a counterclockwise direction on the plane when viewed from the positive direction defined on ℓ (see Fig. 2a). It may be noted that the turn angle of **P** is not uniquely determined. In fact if ρ is a turn angle for **P**, then so is $\rho + k(360°)$ where k is any integer. Hence, any specific value for ρ is merely a representative of the turn angle of **P**. For example, the rotations about the line ℓ with turn angles 240° and −120°, respectively, are really the same rotation **P** with two different turn-angle representations. The identity can be viewed as a rotation whose turn angle is zero (or a multiple of 360°) and whose rotation axis may be considered non-existent or chosen arbitrarily, whichever is more convenient to the situation at hand. It should be stressed again that all of the rotations considered in this paper have axes that pass through $\underrightarrow{O}$.

If we are given any two point isometries $\boldsymbol{\Theta}$ and $\boldsymbol{\Phi}$, we may define a new mapping called the *composition (or product) of* $\boldsymbol{\Theta}$ *and* $\boldsymbol{\Phi}$ denoted by $\boldsymbol{\Theta\Phi}$ and defined by $\boldsymbol{\Theta\Phi}(\underrightarrow{r}) = \boldsymbol{\Theta}(\boldsymbol{\Phi}(\underrightarrow{r}))$ for all $\underrightarrow{r} \in \mathsf{R}^3$. It can be shown that $\boldsymbol{\Theta\Phi}$ is a point isometry. Likewise, it can be shown that the composition of point isometries is *associative, i.e.,* $\boldsymbol{\Theta}(\boldsymbol{\Phi\Psi}) = (\boldsymbol{\Theta\Phi})\boldsymbol{\Psi}$ for all point isometries $\boldsymbol{\Theta}$, $\boldsymbol{\Phi}$ and $\boldsymbol{\Psi}$. It can also be shown that corresponding to each point isometry $\boldsymbol{\Theta}$ there exists a unique point isometry $\boldsymbol{\Phi}$ such that $\boldsymbol{\Theta\Phi} = \boldsymbol{\Phi\Theta} = \boldsymbol{I}$. In this case $\boldsymbol{\Phi}$ is called the *inverse of* $\boldsymbol{\Theta}$ and is denoted by $\boldsymbol{\Phi} = \boldsymbol{\Theta}^{-1}$. By unique we mean that if $\boldsymbol{\Theta\Phi} = \boldsymbol{\Phi\Theta} = \boldsymbol{I}$ and $\boldsymbol{\Theta\Psi} = \boldsymbol{\Psi\Theta} = \boldsymbol{I}$, then $\boldsymbol{\Phi} = \boldsymbol{\Psi}$. The existence of inverses implies the *cancellation law* which states that if **A**, **B** and $\boldsymbol{\Omega}$ are any three point isometries such that $\mathbf{AB} = \mathbf{A\Omega}$, then $\mathbf{B} = \boldsymbol{\Omega}$. If $\mathbf{P}_1$ and $\mathbf{P}_2$ are rotations about the same rotation axis ℓ with turn angles ρ_1 and ρ_2, respectively, then the composition $\mathbf{P}_2\mathbf{P}_1$ is simply the rotation about ℓ with a turn angle of $\rho_1 + \rho_2$. In particular, if $\rho_1 = -\rho_2$, then $\mathbf{P}_2\mathbf{P}_1$ has a turn angle of zero and so $\mathbf{P}_2\mathbf{P}_1 = \boldsymbol{I}$ (*i.e.*, $\mathbf{P}_2 = \mathbf{P}_1^{-1}$). Hence, by the uniqueness of an inverse, the inverse of a rotation is a rotation. It can be shown that the composition of any two rotations (possibly with distinct rotation axes) is again a rotation (see Seitz, 1935). Since this last result is intuitively obvious and because the proof does not contribute to an understanding of the subject under consideration, it will not be given here.

Proper and improper rotations.

In this section we will show that every point isometry is either a rotation or a *rotoinversion,* this latter being the composition of a rotation with a special isometry called the inversion, as defined below. Let $\boldsymbol{\Phi}$ denote a point isometry. We recall from property (4) of a point isometry that the image of every vector under $\boldsymbol{\Phi}$ is completely determined by $\boldsymbol{\Phi}(\underrightarrow{i})$, $\boldsymbol{\Phi}(\underrightarrow{j})$ and $\boldsymbol{\Phi}(\underrightarrow{k})$, the images of the basis vectors under $\boldsymbol{\Phi}$. In Figure 3(a) we have depicted the images of $\underrightarrow{i}$, $\underrightarrow{j}$ and $\underrightarrow{k}$ under $\boldsymbol{\Phi}$. Since $\boldsymbol{\Phi}$ is a point isometry and so

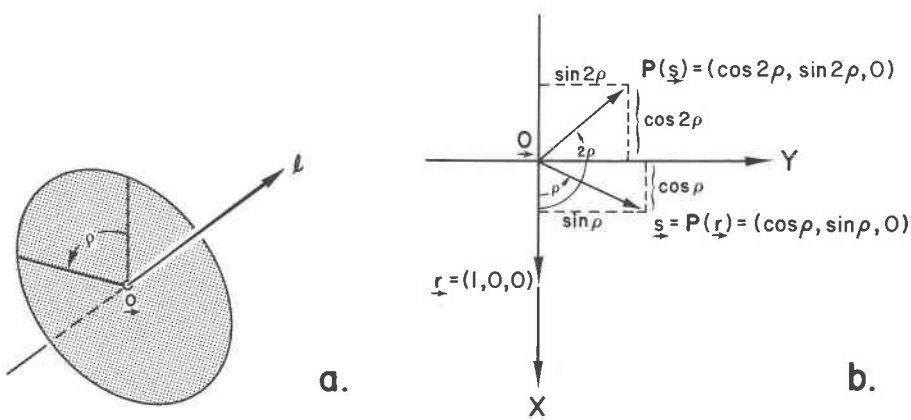

FIG. 2. (a) Diagram showing how the turn angle ρ of the rotation isometry **P** is measured with respect to the rotation axis ℓ; (b) a drawing of the bases vectors $\{r,s\}$ of Γ' viewed down the rotation axis of **P** where Γ' is the set of all vectors in Γ perpendicular to the axis of **P**. It is assumed without loss of generality that the unit length along the X axis is $||\underrightarrow{r}||$. The vector $\underrightarrow{s}$ is the image of $\underrightarrow{r}$ under **P**. Accordingly, $\underrightarrow{s}$ lies in the XY plane, making an angle of ρ with respect to X. Because $\mathbf{P}(\underrightarrow{s}) = \mathbf{P}(\mathbf{P}(\underrightarrow{r})) = \mathbf{P}^2(\underrightarrow{r})$ and because $\mathbf{P}^2$ defines a rotation of 2ρ about Z, $\mathbf{P}(\underrightarrow{s})$ must lie in the XY plane, making an angle of 2ρ with respect to the positive X axis. Since **P** leaves Γ invariant, $\mathbf{P}(\underrightarrow{s}) \in \Gamma$ and so $\mathbf{P}(\underrightarrow{s}) \in \Gamma'$. Since $\underrightarrow{r}$ and $\underrightarrow{s}$ are bases vectors for Γ' and since $\mathbf{P}(\underrightarrow{s}) \in \Gamma'$, $\mathbf{P}(\underrightarrow{s}) = u\underrightarrow{r} + v\underrightarrow{s}$ for some integers u and v.

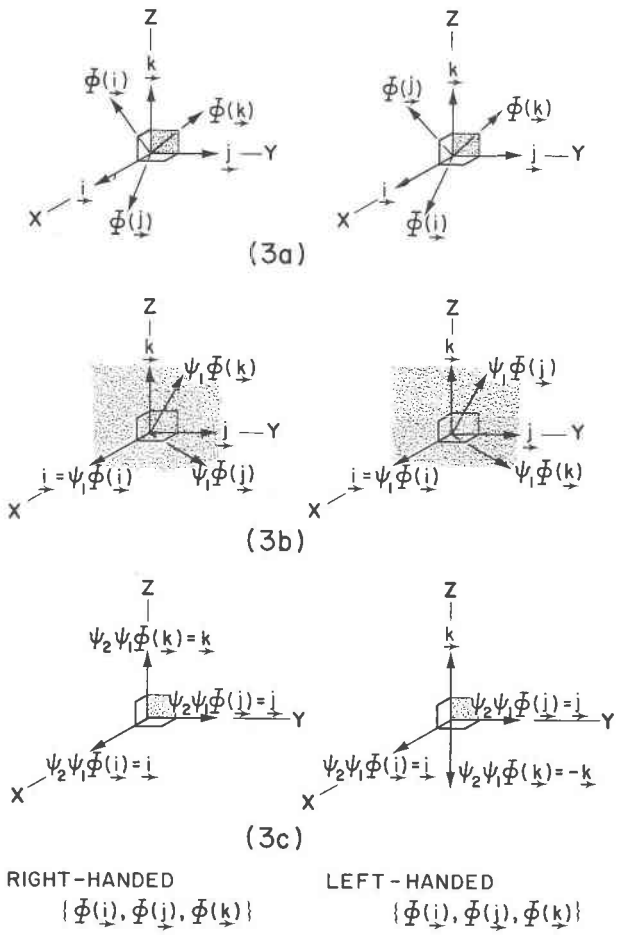

FIG. 3. Given a point isometry Φ, either $\{\Phi(\vec{i}), \Phi(\vec{j}), \Phi(\vec{k})\}$ forms a right-handed coordinate system (depicted in the left column) or a left-handed one (depicted in the right column). (a) shows the original positions of $\Phi(\vec{i})$, $\Phi(\vec{j})$, and $\Phi(\vec{k})$. (b) shows the result of applying Ψ_1 to $\Phi(\vec{i})$, $\Phi(\vec{j})$, and $\Phi(\vec{k})$. The rotation Ψ_1 was chosen to map $\Phi(\vec{i})$ to $\vec{i}$ whereupon $\Phi(\vec{j})$ and $\Phi(\vec{k})$ map into the ZY (stippled) plane; such a rotation can be constructed by using as the rotation axis the line through the origin perpendicular to a plane determined by $\vec{i}$ and $\Phi(\vec{i})$. The turn angle of Ψ_1 is simply the angle between $\vec{i}$ and $\Phi(\vec{i})$. (c) shows the result of applying Ψ_2 to $\Psi_1\Phi(\vec{i})$, $\Psi_1\Phi(\vec{j})$, and $\Psi_1\Phi(\vec{k})$. The rotation Ψ_2 was chosen to map $\Psi_1\Phi(\vec{j})$ to $\vec{j}$. Note that Ψ_2 is constructed in the same way as was Ψ_1 in (3b). Since $\vec{i}$ is perpendicular to a plane containing $\Psi_1\Phi(\vec{j})$ and $\vec{j}$, the rotation axis of Ψ_2 can always be chosen to be the X axis. Hence $\Psi_2\Psi_1\Phi(\vec{i}) = \vec{i}$.

preserves magnitudes and angles, $\{\Phi(\vec{i}),\Phi(\vec{j}),\Phi(\vec{k})\}$ also forms a set of three vectors of unit length which are mutually perpendicular. We will analyze Φ (Fig. 3a) by considering two consecutive rotations Ψ_1 followed by Ψ_2 such that Ψ_1 maps $\Phi(\vec{i})$ to $\vec{i}$—whereupon $\Psi_1(\Phi(\vec{j}))$ and $\Psi_1(\Phi(\vec{k}))$ must lie in the YZ plane (Fig. 3b)—and Ψ_2 is the rotation about the X axis that maps $\Psi_1(\Phi(\vec{j}))$ to $\vec{j}$ and, since its rotation axis is the X axis, leaves $\Psi_1\Phi(\vec{i})$, which is equal to $\vec{i}$ unmoved. Hence $\Psi_2\Psi_1(\Phi(\vec{i})) = \vec{i}$ and $\Psi_2\Psi_1(\Phi(\vec{j})) = \vec{j}$ (Fig. 3c). It was pointed out above that the composition of two consecutive rotations is again a rotation. Accordingly, $\Psi_2\Psi_1$ is a rotation which for convenience we will label Ψ. From above, it therefore follows that $\Psi\Phi(\vec{i}) = \vec{i}$ and $\Psi\Phi(\vec{j}) = \vec{j}$. Two cases are possible for the image of $\Phi(\vec{k})$ under Ψ, namely $\Psi\Phi(\vec{k}) = \vec{k}$ or $\Psi\Phi(\vec{k}) = -\vec{k}$ (see Fig. 3c). We first consider the case where $\Psi\Phi(\vec{k}) = \vec{k}$. Because $\Psi\Phi(\vec{i}) = \vec{i} = I(\vec{i})$, $\Psi\Phi(\vec{j}) = \vec{j} = I(\vec{j})$ and $\Psi\Phi(\vec{k}) = \vec{k} = I(\vec{k})$, we see that $\vec{i}, \vec{j}$, and $\vec{k}$ have the same images under $\Psi\Phi$ as they do under I. Hence we conclude that $\Psi\Phi = I$. Accordingly, Φ is the inverse of a rotation; this, as previously noted, implies that Φ is a rotation. Next we consider the case where $\Psi\Phi(\vec{k}) = -\vec{k}$. By performing a half-turn 2 (a rotation with a turn angle of 180°) about the Z axis, we have $2\Psi\Phi(\vec{i}) = -\vec{i}$, $2\Psi\Phi(\vec{j}) = -\vec{j}$ and $2\Psi\Phi(\vec{k}) = -\vec{k}$. Hence, the isometry $2\Psi\Phi$ maps $\vec{r}$ to $-\vec{r}$ for all $\vec{r}$ in R^3. We call this mapping the *inversion* denoted by i (*i.e.*, $i(\vec{r}) = -\vec{r}$ for all $\vec{r} \in \mathsf{R}^3$). Now $2\Psi\Phi = i$ and so $\Phi = (2\Psi)^{-1}i$ is the composition of the rotation $(2\Psi)^{-1}$ and the inversion, i. A point isometry formed by the composition of a rotation and the inversion is called a *rotoinversion*. We have just shown that every point isometry is either a rotation or a rotoinversion. Since a rotoinversion maps a right-handed coordinate system into a left-handed one (and vice versa), it is often referred to as an *improper rotation*. On the other hand, because rotations do not change the hand of the system, they are sometimes referred to as *proper rotations*. We have also shown that, if Φ is an improper rotation, then there exists a proper rotation P such that $\Phi = \mathrm{P}i$. Since $\mathrm{P}i(\vec{r}) = \mathrm{P}(-\vec{r}) = \mathrm{P}((-1)\vec{r}) = -\mathrm{P}(\vec{r})$ for all $\vec{r} \in \mathsf{R}^3$ and since $i\mathrm{P}(\vec{r}) = i(\mathrm{P}(\vec{r})) = -\mathrm{P}(\vec{r})$ for all $\vec{r} \in \mathsf{R}^3$, we see that $\mathrm{P}i = i\mathrm{P}$ and so i commutes with every proper rotation.

Space lattices

A crystallographic point group consists of a set of point isometries that leave a given space lattice invariant. A subset Γ of R^3 is a space lattice if and only if there exist three non-coplanar vectors $\vec{t}_1$, $\vec{t}_2$ and $\vec{t}_3$ such that

$$\Gamma = \{u\vec{t}_1 + v\vec{t}_2 + w\vec{t}_3 \mid u, v, w \in \mathsf{Z}\}$$

where Z denotes the integers (*i.e.*, $\mathsf{Z} = \{\cdots, -2, -1, 0, 1, 2, \cdots\}$). Notice that in the definition of Γ only integers are allowed as coefficients of $\vec{t}_1$, $\vec{t}_2$, and $\vec{t}_3$, whereas in the definition of R^3 any real number can

serve as a coefficient of i, j, or k. The set $\{\vec{t}_1, \vec{t}_2, \vec{t}_3\}$ is a *basis* for Γ because each vector $\vec{t}$ in Γ may be written as an *integral combination* of $\vec{t}_1$, $\vec{t}_2$, and $\vec{t}_3$, *i.e.*, $\vec{t} = u\vec{t}_1 + v\vec{t}_2 + w\vec{t}_3$ such that u, v, and w are integers. We visualize Γ as the collection of points (called lattice points) in space consisting of the end-points of vectors in Γ radiating from the origin, $\vec{O}$. As stated before, we will not distinguish between a vector and its corresponding lattice point.

Lattice invariant isometries

If Φ is a point isometry, then we say that Γ is invariant under Φ in case $\Gamma = \Phi(\Gamma)$ where we define $\Phi(\Gamma) = \{\Phi(\vec{t}) \mid \vec{t} \in \Gamma\}$; that is, $\Phi(\Gamma)$ is the set of all $\Phi(\vec{t})$ such that $\vec{t}$ is an element of Γ. This is not to say that $\vec{t} = \Phi(\vec{t})$ for all $\vec{t} \in \Gamma$ but merely that Γ and $\Phi(\Gamma)$ are equal sets of vectors. In other words the vectors in Γ are permuted by Φ. Since $\{\vec{t}_1, \vec{t}_2, \vec{t}_3\}$ are non-coplanar, every vector $\vec{r}$ in R^3 is a linear combination of $\{\vec{t}_1, \vec{t}_2, \vec{t}_3\}$, *i.e.*, there exist real numbers p, q, and s such that $\vec{r} = p\vec{t}_1 + q\vec{t}_2 + s\vec{t}_3$. Therefore, $\Phi(\vec{r}) = \Phi(p\vec{t}_1 + q\vec{t}_2 + s\vec{t}_3) = p\Phi(\vec{t}_1) + q\Phi(\vec{t}_2) + s\Phi(\vec{t}_3)$ and so, as in the case of $\{\vec{i},\vec{j},\vec{k}\}$ noted earlier, we see that Φ is completely determined by the images $\{\Phi(\vec{t}_1), \Phi(\vec{t}_2), \Phi(\vec{t}_3)\}$ (Note that the property $\Phi(\Gamma) = \Gamma$ was not required to make this last conclusion. In fact, the conclusion is true for any linear transformation).

We will now show that there is only a finite number of distinct point isometries that leave a given lattice Γ invariant. Consider a sphere S centered at $\vec{O}$ with a large enough radius so that S contains all three of the basis vectors $\vec{t}_1$, $\vec{t}_2$, and $\vec{t}_3$ of Γ and let Φ be an element of the set K of all point isometries that leave the lattice Γ invariant. Since Φ does not stretch vectors (magnitudes are preserved), $\Phi(\vec{t}_1)$, $\Phi(\vec{t}_2)$ and $\Phi(\vec{t}_3)$ must be vectors in Γ that are contained within the sphere. Moreover, since the radius of the sphere is finite, we may assume that there is only a finite number of lattice points of Γ in the sphere (a rigorous proof of this intuitively obvious fact is given in a paper on the derivation of the 14 Bravais lattices being prepared by Boisen and Gibbs). Consequently, there are only a finite number of choices for $\Phi(\vec{t}_1)$, $\Phi(\vec{t}_2)$, and $\Phi(\vec{t}_3)$, *i.e.*, there are only a finite number of possibilities for the images of the vectors $\vec{t}_1$, $\vec{t}_2$, and $\vec{t}_3$ under Φ. Since, as previously observed, Φ is completely determined by $\{\Phi(\vec{t}_1), \Phi(\vec{t}_2), \Phi(\vec{t}_3)\}$, we conclude that there is only a finite number of distinct point isometries in K (*i.e.*, that leave Γ invariant).

Now we consider the algebraic properties of the set of all point isometries K that leave a lattice Γ invariant. The following facts are observed about K:

(1) *Closure*: If $\Phi,\Theta \in$ K, then $\Phi\Theta \in$ K. (This can be seen by observing that $\Phi\Theta(\Gamma) = \Phi(\Theta(\Gamma)) = \Phi(\Gamma) = \Gamma$.)

(2) *Associative law*: If $\Phi,\Theta,\Psi \in$ K, then $\Phi(\Theta\Psi) = (\Phi\Theta)\Psi$. (This was observed earlier.)

(3) *Existence of an identity element:* There exists an element $I \in$ K such that $I\Theta = \Theta I = \Theta$ for all $\Theta \in$ K. (The identity mapping discussed earlier has this property and is in K because $I(\Gamma) = \Gamma$ (in fact, $I(\vec{t}) = \vec{t}$ for all $\vec{t} \in \Gamma$).)

(4) *Existence of an inverse for each element:* Given an element $\Phi \in$ K, there exists an element $\Phi^{-1} \in$ K such that $\Phi\Phi^{-1} = \Phi^{-1}\Phi = I$. (We have observed earlier that the point isometry Φ^{-1} exists. Furthermore, $\Phi^{-1} \in$ K since $\Phi^{-1}(\Gamma) = \Phi^{-1}(\Phi(\Gamma)) = \Phi^{-1}\Phi(\Gamma) = I(\Gamma) = \Gamma$.)

Any set of elements together with a composition obeying the four axioms listed above is an algebraic system called a *group*. Hence K is a group, and since it has only a finite number of elements, it is said to be a *finite group*. The number of elements N in K is called the *order* of K and is designated by $N = \#(K)$. The observation that K is a finite group is important because in general if H is a finite non-empty subset of a group G, then H is itself a group (under the composition of G) if and only if it satisfies the closure axiom (Herstein, 1964). When a subset H of G is a group under the operation of G, we call H a *subgroup* of G. Hence, a nonempty subset H of the finite group G is a subgroup of G if and only if $h_1h_2 \in$ H for all $h_1,h_2 \in$ H. Consequently, if T is any nonempty set of point isometries that leave the lattice Γ invariant, then, since T is a subset of the finite group K, we need only show closure to demonstrate that T is a group. To distinguish these groups from groups of point isometries in general, we call such groups *crystallographic point groups* if a space lattice is left invariant under every element of the group. (Note that the crystallographic point groups are special because, in general, given a point group G there may not exist such a lattice). Moreover, if all of the elements of the group are proper rotations we call it a *proper crystallographic point group*. An *improper crystallographic point group* is one that contains at least one improper rotation.

Possible turn angles for lattice invariant isometries

Let P denote a rotation that leaves a lattice Γ invariant. For convenience, we will choose as its turn angle representative an angle ρ such that $-180° < \rho$

$\leq 180°$. It is proven in a number of places that since P leaves Γ invariant, the only possible turn angle representatives of ρ must be one of the angles $0°$, $\pm 60°$, $\pm 90°$, $\pm 120°$, $180°$ (see for a matrix argument, Seitz, 1935; Burckhardt, 1947; Lomont, 1959; and Janssen, 1973; and see, for a geometric argument, Hilton, 1903; Robertson, 1953; Buerger, 1963; and Bloss, 1971). We will present a new and different proof of this fundamental property of a rotation that leaves a lattice invariant. First we observe that in the case of any such non-identity rotation, P, there must exist a two-dimensional sublattice Γ' of Γ in the plane perpendicular to the rotation axis of P (*cf* Seitz, 1935; Zachariasen, 1945; and Boisen and Gibbs, in preparation). Boisen and Gibbs show that if $\vec{r}$ is a shortest nonzero vector in Γ' and if $\vec{s}$ is a shortest nonzero vector in Γ' noncollinear with $\vec{r}$, then the set $\{\vec{r},\vec{s}\}$ serves as basis generating Γ', that is $\Gamma' = \{u\vec{r} + v\vec{s} \mid u,v \in \mathbf{Z}\}$ (the fact that such vectors $\vec{r}$ and $\vec{s}$ exist is also shown by Boisen and Gibbs). Let $\vec{r}$ be a shortest nonzero vector in Γ'. Without loss of generality, we may place the X axis of our cartesian coordinate system along $\vec{r}$ and the Z axis along the rotation axis of P since it is perpendicular to Γ'. This situation is shown in Figure 2b. If we define the unit length along the X axis to be $\|\vec{r}\|$, then $\vec{r} = (1,0,0)$. Let $\vec{s}$ be the image of $\vec{r}$ under P, that is $\mathbf{P}(\vec{r}) = \vec{s}$. Hence, $\vec{s} \in \Gamma'$, and $\|\vec{r}\| = \|\vec{s}\|$. If the turn-angle of P is $0°$ or $180°$, then ρ is one of the possible turn angle representatives enumerated above and we would be done. On the other hand, if ρ is not equal to $0°$ or $180°$, then $\vec{r}$ and $\vec{s}$ are not collinear and $\vec{s}$, being the same length as $\vec{r}$, is clearly a shortest non-zero vector in Γ' non-collinear with $\vec{r}$. Hence, $\vec{r}$ and $\vec{s}$ constitute a basis for Γ' and each vector $\vec{t} \in \Gamma'$ must be an integral combination of $\vec{r}$ and $\vec{s}$, *i.e.*, $\vec{t} = u\vec{r} + v\vec{s}$ where u and v are integers.

TABLE 1. Symbols and Names for Rotations Associated with the Eight Possible Turn Angles

Turn angle ρ	Symbol for rotation associated with turn angle	Name of rotation
180°	2	half-turn
120°	3	third-turn
90°	4	quarter-turn
60°	6	sixth-turn
0	1	identity
−60°	6^{-1}	negative sixth-turn
−90°	4^{-1}	negative quarter-turn
−120°	3^{-1}	negative third-turn

Then, as demonstrated in Figure 2b, $\vec{s} = (\cos\rho, \sin\rho, 0)$ and $\mathbf{P}(\vec{s}) = (\cos 2\rho, \sin 2\rho, 0)$. Since $\mathbf{P}(\vec{s}) \in \Gamma'$, it must be an integral combination of $\{\vec{r},\vec{s}\}$, *i.e.*, $\mathbf{P}(\vec{s}) = u\vec{r} + v\vec{s}$ where u and v are integers. Therefore,

$$(\cos 2\rho, \sin 2\rho, 0) = u(1, 0, 0) + v(\cos\rho, \sin\rho, 0)$$
$$= (u + v\cos\rho, v\sin\rho, 0)$$

from which it follows that $\sin 2\rho = v\sin\rho$. Replacing $\sin 2\rho$ by $2\sin\rho\cos\rho$, we see that $2\sin\rho\cos\rho = v\sin\rho$. Since $\rho \neq 0$ and $\rho \neq 180$, $\sin\rho \neq 0$ and so $\cos\rho = v/2$. Because $\cos\rho$ is a function bounded by ± 1 and v is an integer, the only possible solutions are $\cos\rho = 0$, $\pm 1/2$, ± 1. Hence ρ is one of the following eight possible turn angles: 0, $\pm 60°$, $\pm 90°$, $\pm 120°$, $180°$. Recall that a positive ρ angle is measured in a counterclockwise direction. The symbol and name corresponding to the rotations associated with each of the eight turn angles are given in Table 1.

The symbols listed in the table describe only the turn angles of corresponding rotations but lack information about the orientation of the rotation axis. Hence, when specifying a non-identity rotation using this symbolism, a description of the orientation of the rotation axis is required. When discussing a point group that leaves a particular lattice Γ invariant, it is customary to choose a conventional unit cell (Table 2.2.2, *International Tables*, vol. I) outlined by the cell edge vectors $\{\vec{a},\vec{b},\vec{c}\}$ (note that $\{\vec{a},\vec{b},\vec{c}\}$ is not always chosen to be a primitive triplet; that is $\{\vec{a}, \vec{b}, \vec{c}\}$ is sometimes not a basis for Γ). The conventional choice of $\vec{a}$, $\vec{b}$, and $\vec{c}$ (Table 2.3.1, *International Tables*, vol. I) turns out to be such that if ℓ is the axis of a rotation that leaves Γ invariant, then there exists a vector $\vec{r} = u\vec{a} + v\vec{b} + w\vec{c}$ along ℓ such that u, v, and w are integers (see Zachariasen, 1945; Buerger, 1963). Since the components u,v,w, of $\vec{r}$ completely define the orientation of the rotation axis with respect to $\{\vec{a},\vec{b},\vec{c}\}$, $[uvw]$ will be used as a left superscript on the rotation symbol to specify the orientation of the rotation axis. Hence, ${}^{[uvw]}\boldsymbol{n}$ where $\boldsymbol{n} = \boldsymbol{2}, \boldsymbol{3}, \boldsymbol{4}$, or $\boldsymbol{6}$ symbolizes a $1/n$ turn about the line $u\vec{a} + v\vec{b} + w\vec{c}$. Thus, ${}^{[100]}\boldsymbol{2}$ symbolizes a half-turn parallel to $\vec{a}$, ${}^{[010]}\boldsymbol{4}$ symbolizes a quarter-turn parallel to $\vec{b}$ whereas ${}^{[\bar{1}11]}\boldsymbol{3}^{-1}$ symbolizes a negative third-turn parallel to $-\vec{a}-\vec{b}+\vec{c}$. The one exception to our rule is when the rotation axis parallels $-\vec{c}$; in that case no orientation symbol is attached to the rotation symbol, hence $\boldsymbol{4}^{-1}$ denotes a negative quarter-turn about $\vec{c}$. We will always place the Z axis of our cartesian coordinate system along $\vec{c}$. For groups requiring orientation symbols, $\vec{a}$ and $\vec{b}$ will be chosen so that they are perpendicular to $\vec{c}$ and X will be chosen to lie

along $\underrightarrow{a}$. (The fact that $\underrightarrow{a}$ and $\underrightarrow{b}$ can be placed perpendicular to $\underrightarrow{c}$ is not obvious and is explored by Seitz, 1935, and Boisen and Gibbs, in preparation.)

As observed earlier, if Φ denotes a rotoinversion, then $\Phi = \mathbf{P}i$ for some proper rotation P. We will assign as the turn angle of Φ the turn angle of P and as the rotation axis of Φ the rotation axis of P. Hence the orientation symbol for Φ is the orientation symbol for P. The names and symbols for the rotoinversions corresponding to the eight possible turn angles are given in Table 2. Note that $2i = \bar{2}$ can also be visualized as a reflection denoted by m, where m refers to the mirror plane about which the reflection occurs. The orientation symbol given to m is inherited from the half-turn perpendicular to the mirror plane. For example, $^{[100]}m$ denotes a reflection whose mirror plane is perpendicular to $\underrightarrow{a}$ while m denotes a reflection whose mirror plane is perpendicular to $\underrightarrow{c}$.

Proper crystallographic point groups

If G is a finite group consisting of rotations of the type listed in Table 1, then G may be shown to leave some lattice Γ invariant (Boisen and Gibbs, in preparation). Consequently, the search for proper crystallographic point groups is equivalent to the search for those finite groups consisting of rotations of the type listed in Table 1. When all of the rotations of G have the same rotation axis, we call G a *proper monaxial group*. When G has two or more rotations with distinct axes, then we call G a *proper polyaxial group*.

Proper monaxial groups

It is evident that each of the following collections of crystallographic rotations $\{1\}$, $\{2,1\}$, $\{3,3^{-1},1\}$, $\{4,2,4^{-1}, 1\}$, and $\{6,3,2,3^{-1}, 6^{-1},1\}$ forms a proper monaxial group where all of the rotations in each collection take place about the same axis. (Recall we need only demonstrate closure to conclude that each is a group. For example, for $\{3,3^{-1},1\}$ we observe that each of compositions $33 = 3^{-1}$, $33^{-1} = 1$, $31 = 3$, $3^{-1}3 = 1$, $3^{-1}3^{-1} = 3$, $3^{-1}1 = 3^{-1}$, $13 = 3$, $13^{-1} = 3^{-1}$ and $11 = 1$ is in $\{3, 3^{-1}, 1\}$ and so we have demonstrated closure for $\{3, 3^{-1}, 1\}$.) The list of monaxial groups given above exhausts those that can be made from the rotations presented in Table 1. This can be quickly checked by considering each of the remaining collections and showing that no other such group is possible (*e.g.*, $\{1,2,3\}$ is not closed because $23 = 6^{-1} \notin \{1,2,3\}$). Since $\{6,3,2,3^{-1},6^{-1},1\} = \{6,6^2,6^3,6^4,6^5,6^6\}$, we call $\{6,3,2,3^{-1},6^{-1},1\}$ a cyclic group generated by 6. In group theoretic notation we write $\langle 6\rangle = \{6,6^2, 6^3,6^4,6^5,6^6\} = \{6,3,2,3^{-1},6^{-1},1\}$ and denote the group by 6. Note that $\langle 6^{-1}\rangle = \{6^{-1},6^{-2},6^{-3},6^{-4},6^{-5},6^{-6}\} = \{6^{-1},3^{-1},2,3,6,1\}$. Since the order of listing the elements is immaterial, we see that $\langle 6\rangle = \langle 6^{-1}\rangle$ and hence 6^{-1} is another generator of the group 6. A similar situation exists for the other monaxial groups as evinced by Table 3. In summary, we have shown that all of the proper monaxial crystallographic point groups are cyclic. Because of theoretical considerations used later in this paper, we require a more formal definition of a cyclic group. A group G is a *cyclic group* if and only if there exists an element $g \in$ G such that $\mathrm{G} = \langle g\rangle = \{g^n | n \in \mathrm{Z}\}$. Here g is referred to as the *generator* of the group. In the case where G is a finite group it is sufficient to consider only the positive powers of the generator as borne out by our examples above. In fact, if $\langle g\rangle$ is finite and $t = \#(\langle g\rangle)$, then t is the smallest positive integer such that $g^t = 1$. For example, in the case of $\langle 4^{-1}\rangle$, the smallest positive integer t such that $(4^{-1})^t = 1$ is $t = 4$, hence $\#(\langle 4^{-1}\rangle) = 4$ as evinced by Table 3. As seen in Table 3, there is only one distinct monaxial group of each order about a single axis. If G is a proper monaxial group of order n, then we will use the symbol n to

TABLE 2. Names and Symbols for the Rotoinversions Associated with the Eight Turn Angles

Turn angle ρ	Symbol for rotoinversion associated with turn angle	Name of rotoinversion
180°	$m = i2 = 2i = \bar{2}$	reflection
120°	$\bar{3} = i3 = 3i$	third-turn inversion
90°	$\bar{4} = i4 = 4i$	quarter-turn inversion
60°	$\bar{6} = i6 = 6i$	sixth-turn inversion
0	$i = i1 = 1i = \bar{1}$	inversion
−60°	$\bar{6}^{-1} = i6^{-1} = 6^{-1}i$	negative sixth-turn inversion
−90°	$\bar{4}^{-1} = i4^{-1} = 4^{-1}i$	negative quarter-turn inversion
−120°	$\bar{3}^{-1} = i3^{-1} = 3^{-1}i$	negative third-turn inversion

TABLE 3. The Proper Monaxial Groups, Their Generators and Elements

Group symbol	Group generators and elements
1	$\langle 1\rangle = \{1\}$
2	$\langle 2\rangle = \{1, 2\}$
3	$\langle 3\rangle = \langle 3^{-1}\rangle = \{1, 3, 3^{-1}\}$
4	$\langle 4\rangle = \langle 4^{-1}\rangle = \{1, 4, 2, 4^{-1}\}$
6	$\langle 6\rangle = \langle 6^{-1}\rangle = \{1, 6, 3, 2, 3^{-1}, 6^{-1}\}$

designate the point group. The axis common to all of the rotations of a given monaxial group n (where n = 2, 3, 4, or 6) will be called an *n-fold axis.* (When n is different from 1, 2, 3, 4, and 6, a perfectly good point group results in the manner described above. However, for such a point group no space lattice is left invariant and hence it is not a crystallographic point group.)

Proper polyaxial groups

In our investigation of the polyaxial groups, we will be examining combinations of monaxial groups. The task of finding the possible proper polyaxial point groups will be considerably more difficult than that of finding the monaxial point groups. It will require some fairly sophisticated arguments and a considerable amount of notation which will be explained as we go along. The main aim of this section is to establish the inequality which in loose terms will state that three monaxial groups with orders ν_1, ν_2, and ν_3, respectively, may be used to form a proper polyaxial point group only if

$$1/\nu_1 + 1/\nu_2 + 1/\nu_3 > 1.$$

To facilitate our proof that will establish this inequality we will consider the surface $\mathbb{S}$ of a unit sphere centered at $\vec{O}$. Any point isometry Φ acting on $\mathbb{S}$ maps $\mathbb{S}$ onto itself. In fact, Φ is completely determined by its action on $\mathbb{S}$ because the effect of Φ on $\mathbb{S}$ determines the end-points of $\Phi(\vec{i})$, $\Phi(\vec{j})$ and $\Phi(\vec{k})$ and therefore the components of $\Phi(\vec{i})$, $\Phi(\vec{j})$ and $\Phi(\vec{k})$. A non-identity proper rotation $\boldsymbol{h}$ about the rotation axis ℓ leaves exactly two antipodal points on $\mathbb{S}$ unmoved. These points are precisely the points at which ℓ and $\mathbb{S}$ intersect and are called the *pole points* belonging to $\boldsymbol{h}$. If these two points are labelled p and q, then they are the only points x on $\mathbb{S}$ that satisfy the equality $\boldsymbol{h}(x) = x$. Let G be a proper polyaxial group. The trivial group $\boldsymbol{1}$ has already been treated as a monaxial group and since it has no pole points we deliberately exclude it from consideration in the remainder of this discussion. Hence we will assume that #(G) $\geq$ 2. To help illustrate a number of the concepts given below, we will on occasion use the proper polyaxial group 322 as an example. However, none of the theoretical concepts that follow depend on the assumption that 322 exists. The rotations of 322 are $\{\boldsymbol{1},\boldsymbol{3},\boldsymbol{3}^{-1},{}^{[100]}\boldsymbol{2},{}^{[110]}\boldsymbol{2},{}^{[010]}\boldsymbol{2}\}$. Since 322 consists of 6 distinct rotations, by definition #(322) = 6. The orientation of each of these rotations is shown in Figure 4a (recall that the left superscript is only assigned to a rotation symbol when the rotation occurs about an axis other than Z), and the pole points belonging to the rotations of 322 are depicted in Figure 4b. The multiplication table for 322 given in Table 4 serves to define the structure of the group by enumerating the compositions of all possible pairs of group rotations. Since the only rotations that appear in the table are the six rotations already listed for 322, we may conclude that 322 is closed under composition and hence is a group.

TABLE 4. Group Multiplication Table for Group 322

322	$\boldsymbol{1}$	$\boldsymbol{3}$	$\boldsymbol{3}^{-1}$	${}^{[100]}\boldsymbol{2}$	${}^{[110]}\boldsymbol{2}$	${}^{[010]}\boldsymbol{2}$
$\boldsymbol{1}$	$\boldsymbol{1}$	$\boldsymbol{3}$	$\boldsymbol{3}^{-1}$	${}^{[100]}\boldsymbol{2}$	${}^{[110]}\boldsymbol{2}$	${}^{[010]}\boldsymbol{2}$
$\boldsymbol{3}$	$\boldsymbol{3}$	$\boldsymbol{3}^{-1}$	$\boldsymbol{1}$	${}^{[110]}\boldsymbol{2}$	${}^{[010]}\boldsymbol{2}$	${}^{[100]}\boldsymbol{2}$
$\boldsymbol{3}^{-1}$	$\boldsymbol{3}^{-1}$	$\boldsymbol{1}$	$\boldsymbol{3}$	${}^{[010]}\boldsymbol{2}$	${}^{[100]}\boldsymbol{2}$	${}^{[110]}\boldsymbol{2}$
${}^{[100]}\boldsymbol{2}$	${}^{[100]}\boldsymbol{2}$	${}^{[010]}\boldsymbol{2}$	${}^{[110]}\boldsymbol{2}$	$\boldsymbol{1}$	$\boldsymbol{3}^{-1}$	$\boldsymbol{3}$
${}^{[110]}\boldsymbol{2}$	${}^{[110]}\boldsymbol{2}$	${}^{[100]}\boldsymbol{2}$	${}^{[010]}\boldsymbol{2}$	$\boldsymbol{3}$	$\boldsymbol{1}$	$\boldsymbol{3}^{-1}$
${}^{[010]}\boldsymbol{2}$	${}^{[010]}\boldsymbol{2}$	${}^{[110]}\boldsymbol{2}$	${}^{[100]}\boldsymbol{2}$	$\boldsymbol{3}^{-1}$	$\boldsymbol{3}$	$\boldsymbol{1}$

Let p denote a pole point of G. Then the collection of all rotations of G that have p as a pole point is designated by G_p, *i.e.*, $\mathsf{G}_p = \{\boldsymbol{g} \in \mathsf{G} | \boldsymbol{g}(p) = p\}$.* If $\boldsymbol{g}_1, \boldsymbol{g}_2 \in \mathsf{G}_p$, then $\boldsymbol{g}_1\boldsymbol{g}_2(p) = \boldsymbol{g}_1(\boldsymbol{g}_2(p)) = \boldsymbol{g}_1(p) = p$. Since $\boldsymbol{g}_1$ and $\boldsymbol{g}_2$ were arbitrarily chosen rotations of G_p and since $\boldsymbol{g}_1\boldsymbol{g}_2 \in \mathsf{G}_p$, we conclude that G_p is closed under the composition and hence a subgroup of G. Since the rotations of G_p leave p fixed, they all have the line $\vec{O}p$ containing $\vec{O}$ and p as their rotation axis. Consequently, G_p is a proper monaxial group and therefore one of the cyclic groups listed in Table 3.

In the case of 322, $(322)_{p21} = (322)_{p32} = \{{}^{[100]}\boldsymbol{2},\boldsymbol{1}\}$, $(322)_{p31} = (322)_{p23} = \{{}^{[110]}\boldsymbol{2},\boldsymbol{1}\}$, $(322)_{p22} = (322)_{p33} = \{{}^{[010]}\boldsymbol{2},\boldsymbol{1}\}$ and $(322)_{p11} = (322)_{p12} = \{\boldsymbol{3},\boldsymbol{3}^{-1},\boldsymbol{1}\}$. We observe in this example that two pole points are associated with each monaxial group (Fig. 4). It is also evident that the pole points p_{21}, p_{22}, p_{23}, p_{31}, p_{32}, and p_{33} are each associated with the group 2 where the rotation axis of each has a different orientation. The remaining pole points p_{11} and p_{12} are similarly associated with group 3 (see Table 3). (The significance of the double subscripts attached to each pole point belonging to 322 will be discussed later. For the time being, the subscripts may serve to distinguish distinct pole points.)

* The subset G_p of G, consisting of all $\boldsymbol{g} \in \mathsf{G}$ for which $\boldsymbol{g}(p) = p$, is a subgroup of G sometimes called the *stabilizer* of p.

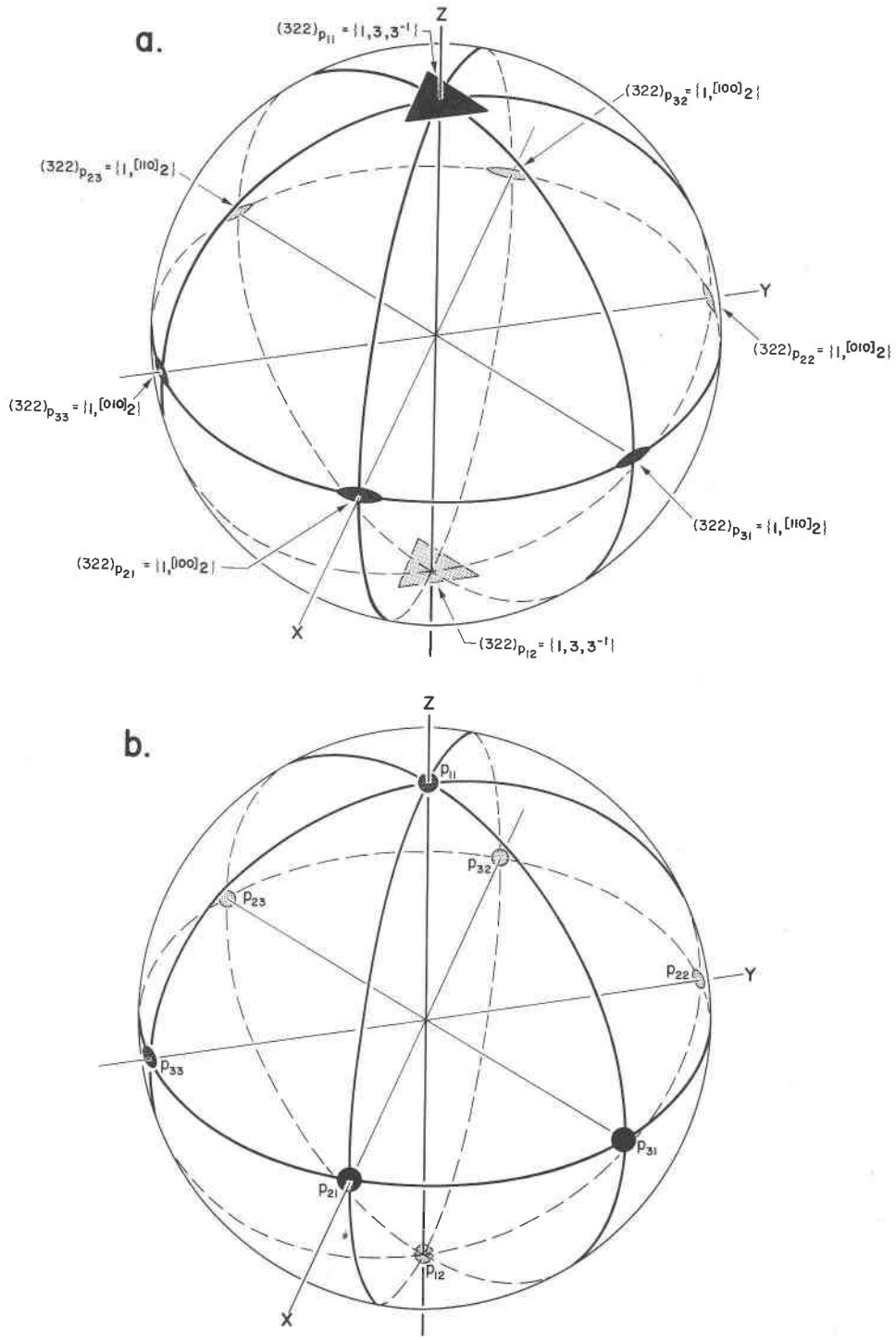

FIG. 4. The orientations of the rotation axes and the associated pole points for point group 322 are shown in (a) and (b), respectively. The bases vectors $\vec{a}, \vec{b}, \vec{c}$ lie along X, Y, and Z, respectively, and so are not shown. Note that in this figure X, Y, and Z are not mutually perpendicular, since the angle between X and Y is 120° (the angles between X and Z and Y and Z are both 90°).

Theorem 1. Let p and q be pole points belonging to the proper polyaxial group G such that there exists a rotation $g \in G$ such that $g(p) = q$. Then the cyclic groups G_p and G_q have the same order; that is $\#(G_p) = \#(G_q)$.**

Proof. From the discussion above we know that G_p and G_q are monaxial and hence cyclic groups. Let h be a generator of G_p and let $n = \#(G_p)$ and $m = \#(G_q)$. We want to show that $m = n$. As observed in the section on proper monaxial groups, n is the smallest positive integer such that $h^n = 1$. Consider the rotation ghg^{-1} where $g(p) = q$ (such a g exists by the hypothesis of the theorem). Since $g^{-1}(q) = p$ and $h(p) = p$, we observe that $ghg^{-1}(q) = g(h(g^{-1}(q))) = g(h(p)) = g(p) = q$. Hence $ghg^{-1}(q) = q$ demonstrating that $ghg^{-1} \in G_q$. We next show that ghg^{-1} is a generator of G_q. Let f be an arbitrary rotation of G_q. Then $g^{-1}fg \in G_p$ because $g^{-1}fg(p) = g^{-1}(f(g(p))) = g^{-1}(f(q)) = g^{-1}(q) = p$. Therefore, since $G_p = \langle h \rangle$, $g^{-1}fg = h^t$ for some integer $1 \leq t \leq n$. Hence $gh^tg^{-1} = g(g^{-1}fg)g^{-1} = f$. Therefore

$$
\begin{aligned}
f &= gh^tg^{-1} \\
&= ghh \cdots hg^{-1} \text{ (where } h \text{ occurs } t \text{ times)} \\
&= gh(g^{-1}g)h(g^{-1}g)h \cdots (g^{-1}g)hg^{-1} \text{ (since } g^{-1}g = 1) \\
&= (ghg^{-1})(ghg^{-1}) \cdots (ghg^{-1}) \text{ (by associative law)} \\
&= (ghg^{-1})^t
\end{aligned}
$$

Consequently f is a power of ghg^{-1}. Since f was an arbitrarily chosen rotation of G_q, we have shown that $G_q = \langle ghg^{-1} \rangle$. Since $m = \#(G_q)$, as observed earlier m is the smallest positive integer such that $(ghg^{-1})^m = 1$. However, since $n = \#(G_p)$, $(ghg^{-1})^n = gh^ng^{-1} = g1g^{-1} = 1$, but m is the smallest such integer hence $m \leq n$. But $(ghg^{-1})^m = gh^mg^{-1} = 1$ and accordingly $h^m = g^{-1}g = 1$. However $n = \#(G_p)$ is the smallest positive integer such that $h^n = 1$. Hence $n \leq m$. Therefore, since $n \leq m$ and $m \leq n$, we conclude that $m = n$ and so $\#(G_p) = \#(G_q)$.

In our example 322, if we consider the cyclic group $(322)_{p_{31}} = \{1, {}^{[110]}2\}$ we see that ${}^{[110]}2(p_{21}) = p_{22}$. Hence, according to Theorem 1 we can conclude that $\#((322)_{p_{21}}) = \#((322)_{p_{22}})$. We observe that this is indeed true because $(322)_{p_{22}} = \{1\, {}^{[010]}2\}$ and hence both sets contain two rotations. Similarly ${}^{[100]}2(p_{11}) = p_{12}$ and therefore we can conclude that $(322)_{p_{11}}$ and $(322)_{p_{12}}$ have the same order. Again an examination of Figure 4 shows this to be the case since $(322)_{p_{11}} = \{1,3,3^{-1}\}$ and $(322)_{p_{12}} = \{1,3,3^{-1}\}$. It may also be predicted from Theorem 1 that there will be no group element in 322 that maps p_{21} to p_{11} because their corresponding groups $(322)_{p_{21}}$ and $(322)_{p_{11}}$ are of different orders. This is easily verified by considering the rotations in 322 one at a time and observing that indeed none of them map p_{21} to p_{11}.

We will now investigate an important relationship that exists between the pole points of any given rotation group G. We define $\mathcal{P}(G)$ to be the set of all pole points belonging to the rotations of G, *i.e.*, $\mathcal{P}(G) = \{p \in \mathcal{S} |$ there exists at least one $g \in G$ such that $g \neq 1$ and $g(p) = p\}$. For example, in the case of 322, $\mathcal{P}(322) = \{p_{11}, p_{12}, p_{21}, p_{22}, p_{23}, p_{31}, p_{32}, p_{33}\}$. We now define a relation on $\mathcal{P}(G)$ by defining for each $p_1, p_2 \in \mathcal{P}(G)$ that p_1 is equivalent to p_2 (symbolized $p_1 \sim p_2$) if and only if there exists a rotation $g \in G$ such that $g(p_1) = p_2$. Hence, if $p_1 \sim p_2$, then from Theorem 1 we know that G_{p_1} and G_{p_2} are cyclic groups of identical orders, *i.e.*, $\#(G_{p_1}) = \#(G_{p_2})$.

We observe the following important properties of $\mathcal{P}(G)$ with respect to the relation defined in the last paragraph:

(1) *Reflexive:* For all $p \in \mathcal{P}(G)$, $p \sim p$. (This is because G has an identity element 1 and $1(p) = p$. Hence $p \sim p$.)

(2) *Symmetric:* For all $p_1, p_2 \in \mathcal{P}(G)$, if $p_1 \sim p_2$, then $p_2 \sim p_1$. (This is because if $g \in G$ such that $g(p_1) = p_2$, then g has an inverse $g^{-1} \in G$ so that $g^{-1}(p_2) = p_1$. Hence $p_2 \sim p_1$.)

(3) *Transitive:* For all $p_1, p_2, p_3 \in \mathcal{P}(G)$, if $p_1 \sim p_2$ and $p_2 \sim p_3$, then $p_1 \sim p_3$. (This is because if $g(p_1) = p_2$ and $h(p_2) = p_3$ where $g, h \in G$, then $hg \in G$ and $hg(p_1) = h(g(p_1)) = h(p_2) = p_3$. Hence $p_1 \sim p_3$.)

Any relation defined on a set satisfying these three properties is called an *equivalence relation.* Let $p \in \mathcal{P}(G)$, then we define the *equivalence class* determined by p to be $[p] = \{q \in \mathcal{P}(G) | p \sim q\}$.* That is, $[p]$ is the set of all pole points of G equivalent to p. Since $p \sim p$, we have $p \in [p]$ and so every element of $\mathcal{P}(G)$ appears in some equivalence class; hence $\mathcal{P}(G)$ is the union** of all of its equivalence classes. Furthermore, if $[p]$ and $[q]$ have one or more elements in common (symbolized by $[p] \cap [q] \neq \emptyset$),*** then $[p] = [q]$.

** Those familiar with group theory will recognize that this theorem shows that G_p is isomorphic to G_q since they are both cyclic.

* The subset of $\mathcal{S}$ consisting of all $g(p)$ as g ranges over all G is sometimes called the *orbit* of p.

** The union of a collection of given sets is the set consisting of all those elements that appear in at least one of the given sets. The union of two sets A and B is symbolized $A \cup B$ and the symbolism $\bigcup_{i=1}^{3} A_i$ means $A_1 \cup A_2 \cup A_3$.

*** The expression "$A \cap B$" denotes the intersection of sets A and B, *i.e.*, the set of all elements that are in both A and B.

The symbol $\emptyset$ denotes the empty set; *i.e.*, the set containing no elements.

Accordingly, distinct classes are disjoint, *i.e.*, they have no elements in common. A thorough discussion of equivalence classes including proofs of our observations above can be found in most modern abstract alegbra texts (*e.g.*, Larsen, 1969; Shapiro, 1975).

In our example of 322, the elements of the equivalence class of p_{21} in $\mathcal{P}(322)$ are $[p_{21}] = \{p_{ij} \in \mathcal{P}(322) \mid p_{21} \sim p_{ij}\} =$
$\{p_{ij} \in \mathcal{P}(322) \mid$ there exists an element $\boldsymbol{g} \in 322$ such that $\boldsymbol{g}(p_{21}) = p_{ij}\}$

$$= \{\boldsymbol{g}(p_{21}) \mid \boldsymbol{g} \in 322\}$$

$$= (\boldsymbol{1}(p_{21}),\ \boldsymbol{3}(p_{21}),\ \boldsymbol{3}^{-1}(p_{21}),\ {}^{[100]}\boldsymbol{2}(p_{21}),\ {}^{[110]}\boldsymbol{2}(p_{21}),\ {}^{[010]}\boldsymbol{2}(p_{21})\}$$

$$= \{p_{21}, p_{22}, p_{23}, p_{21}, p_{22}, p_{23}\}$$

$$= \{p_{21}, p_{22}, p_{23}\}.$$

Following the same procedure one may calculate each of the equivalence classes of $\mathcal{P}(322)$. The results are: $[p_{21}] = [p_{22}] = [p_{23}] = \{p_{21},p_{22},p_{23}\}$, $[p_{31}] = [p_{32}] = [p_{33}] = \{p_{31},p_{32},p_{33}\}$, and $[p_{11}] = [p_{12}] = \{p_{11},p_{12}\}$. We notice that it is indeed true that these equivalence classes are disjoint and that $\mathcal{P}(322)$ is their union. The pole point notation for 322 was deliberately chosen at the outset so that points with the same first subscript would be in the same equivalence class.

Let t denote the number of distinct equivalence classes of $\mathcal{P}(\mathsf{G})$ where $\mathsf{C}_1(\mathsf{G}), \mathsf{C}_2(\mathsf{G}), \cdots, \mathsf{C}_t(\mathsf{G})$ denotes the equivalence classes of $\mathcal{P}(\mathsf{G})$, *i.e.*, $\mathsf{C}_i(\mathsf{G}) = [p]$ for some $p \in \mathcal{P}(\mathsf{G})$, hence

$$\bigcup_{i=1}^{t} \mathsf{C}_i(\mathsf{G}) = \mathcal{P}(\mathsf{G}) \quad \text{and} \quad \mathsf{C}_i(\mathsf{G}) \cap \mathsf{C}_j(\mathsf{G}) = \emptyset \quad \text{if} \quad i \neq j.$$

It should be observed that $\mathcal{P}(\mathsf{G})$ is a finite set because G is a finite set and each non-identity element of G has only two pole points. Hence, each $\mathsf{C}_i(\mathsf{G})$ is a finite set and we let n_i denote the number of points in $\mathsf{C}_i(\mathsf{G})$; that is, $n_i = \#(\mathsf{C}_i(\mathsf{G}))$. Therefore, we may list the elements of $\mathsf{C}_i(\mathsf{G})$ as $p_{i1}, p_{i2}, \cdots, p_{in_i}$. In the case of our example, $\mathsf{C}_1(322) = \{p_{11},p_{12}\}$, $\mathsf{C}_2(322) = \{p_{21},p_{22},p_{23}\}$, and $\mathsf{C}_3(322) = \{p_{31},p_{32},p_{33}\}$ and as observed above, $\mathcal{P}(322) = \bigcup_{i=1}^{3} \mathsf{C}_i(322) = \mathsf{C}_1(322) \cup \mathsf{C}_2(322) \cup \mathsf{C}_3(322)$. In addition, notice that $n_1 = \#(\mathsf{C}_1(322)) = 2$, $n_2 = \#(\mathsf{C}_2(322)) = 3$ and $n_3 = \#(\mathsf{C}_3(322)) = 3$.

Let H_{ij} denote $\mathsf{G}_{p_{ij}}$ the group of all rotations in G that leave p_{ij} fixed. Since p_{ij} and p_{ik} are both in $\mathsf{C}_i(\mathsf{G})$, $\#(\mathsf{H}_{ij}) = \#(\mathsf{H}_{ik})$ because $p_{ij} \sim p_{ik}$ (see Theorem 1). Hence $\mathsf{H}_{i1}, \mathsf{H}_{i2}, \cdots, \mathsf{H}_{in_i}$ all have the same order which we signify as ν_i. It follows that H_{ij} is a cyclic group of order ν_i and if we let h_{ij} be the generator for H_{ij}, then $\mathsf{H}_{ij} = \{h_{ij}, h_{ij}^2, \cdots, h_{ij}^{\nu_i}\}$. Moreover the axis common to the rotations of H_{ij} is a ν_i-fold axis (this axis of course passes through p_{ij} and the origin, O). In the context of our example 322, we see that $\mathsf{H}_{11} = \{\boldsymbol{1},\boldsymbol{3},\boldsymbol{3}^{-1}\}$, $\mathsf{H}_{12} = \{\boldsymbol{1},\boldsymbol{3},\boldsymbol{3}^{-1}\}$, $\mathsf{H}_{21} = \{\boldsymbol{1},{}^{[100]}\boldsymbol{2}\}$, $\mathsf{H}_{22} = \{\boldsymbol{1},{}^{[010]}\boldsymbol{2}\}$, $\mathsf{H}_{23} = \{\boldsymbol{1},{}^{[110]}\boldsymbol{2}\}$, $\mathsf{H}_{31} = \{\boldsymbol{1},{}^{[110]}\boldsymbol{2}\}$, $\mathsf{H}_{32} = \{\boldsymbol{1},{}^{[100]}\boldsymbol{2}\}$, and $\mathsf{H}_{33} = \{\boldsymbol{1}\ {}^{[010]}\boldsymbol{2}\}$. In addition we observed that $\#(\mathsf{H}_{11}) = \#(\mathsf{H}_{12}) = \nu_1 = 3$, $\#(\mathsf{H}_{21}) = \#(\mathsf{H}_{22}) = \#(\mathsf{H}_{23}) = \nu_2 = 2$, and $\#(\mathsf{H}_{31}) = \#(\mathsf{H}_{32}) = \#(\mathsf{H}_{33}) = \nu_3 = 2$.

We are about to present a lengthy derivation of some important relationships between many of the concepts discussed above. These relationships will be used to develop facts about G which will ultimately enable us to determine all of the proper crystallographic point groups which we then list in Table 6. In an attempt to present this discussion in a more understandable fashion, each of the more important relationships will be set off in a box at the beginning of each argument where the relationship is established.

$$\boxed{2(N-1) = \sum_{i=1}^{t} n_i(\nu_i - 1)} \tag{1}$$

Recall that $N = \#(\mathsf{G})$, $\nu_i = \#(\mathsf{H}_{ij})$, $n_i = \#(\mathsf{C}_i(\mathsf{G}))$, and t is the number of equivalence classes of pole points. The basic strategy for establishing Equation (1) will be to find two distinct ways of counting the nonidentity rotations of G. The result will be two expressions each equaling twice the number of nonidentity rotations of G. This will establish Equation (1) since these two equal expressions will be precisely those appearing in the equation. We begin by taking each pole point p_{ij} in $\mathcal{P}(\mathsf{G})$ one at a time and counting the number of non-identity rotations of G leaving p_{ij} fixed. The sum of these numbers taken over all the pole points in $\mathcal{P}(\mathsf{G})$ will equal twice the number of nonidentity rotations in G because each of these rotations leaves exactly two pole points fixed and hence is counted twice. The number of non-identity rotations leaving p_{ij} fixed is $\#(\mathsf{H}_{ij}) - 1 = \nu_i - 1$. Thus, for the pole points in $\mathsf{C}_1(\mathsf{G})$ we have

#(non-identity rotations leaving p_{11} fixed) $= \nu_1 - 1$
#(non-identity rotations leaving p_{12} fixed) $= \nu_1 - 1$
. . .
. . .
. . .
#(non-identity rotations leaving p_{1n_1} fixed) $= \nu_1 - 1$

} n_1 equations

TABLE 5. Display of the Derivation of Equation (1) for Group 322

Notation for group G	Notation for group 322							
$\mathcal{P}(\mathsf{G})$	$\mathcal{P}(322) = \{p_{11}, p_{12}, p_{21}, p_{22}, p_{23}, p_{31}, p_{32}, p_{33}\}$							
$\mathsf{C}_i(\mathsf{G})$	$\mathsf{C}_1(322)$		$\mathsf{C}_2(322)$			$\mathsf{C}_3(322)$		
p_{ij}	p_{11}	p_{12}	p_{21}	p_{22}	p_{23}	p_{31}	p_{32}	p_{33}
$\mathsf{G}_{pij} = \{g \in \mathsf{G} \mid g(p_{ij}) = p_{ij}\}$	$(322)_{p_{11}} = \{1, 3, 3^{-1}\}$	$(322)_{p_{12}} = \{1, 3, 3^{-1}\}$	$(322)_{p_{21}} = \{1, {}^{[100]}2\}$	$(322)_{p_{22}} = \{1, {}^{[010]}2\}$	$(322)_{p_{23}} = \{1, {}^{[110]}2\}$	$(322)_{p_{31}} = \{1, {}^{[110]}2\}$	$(322)_{p_{32}} = \{1, {}^{[100]}2\}$	$(322)_{p_{33}} = \{1, {}^{[010]}2\}$
$(\nu_i - 1)$	$(3-1)$	$(3-1)$	$(2-1)$	$(2-1)$	$(2-1)$	$(2-1)$	$(2-1)$	$(2-1)$
$n_i(\nu_i - 1)$	$2(3-1) = 4$		$3(2-1) = 3$			$3(2-1) = 3$		
$\sum_{i=1}^{t} n_i(\nu_i - 1)$	$4 + 3 + 3 = 10$							
$2(\#(\mathsf{G}) - 1)$	$2(\#(322) - 1) = 2(6-1) = 10$							

Summing up these numbers we find that the contribution from $\mathsf{C}_1(\mathsf{G})$ is $n_1(\nu_1 - 1)$. Following the same argument, we see that the contribution from $\mathsf{C}_i(\mathsf{G})$ is $n_i(\nu_i - 1)$ for each $1 \le i \le t$. Adding the contribution from each of the t equivalence classes, we find that the sum is $\sum_{i=1}^{t} n_i(\nu_i - 1)$. Since $N-1$ is the number of non-identity rotations in G, it follows that twice the number of non-identity rotations in G is $2(N-1)$ and so we have established Equation (1), namely

$$2(N-1) = \sum_{i=1}^{t} n_i(\nu_i - 1). \tag{1}$$

Returning to our example 322, we observed earlier that $N = 6$, $n_1 = 2$, $n_2 = 3$, $n_3 = 3$, $\nu_1 = 3$, $\nu_2 = 2$, and $\nu_3 = 2$. The notation used in the derivation of Equation (1) is displayed for 322 in Table 5. It is clear from the table that, as predicted by Equation (1), $2(\#(322) - 1) = 10 = n_1(\nu_1 - 1) + n_2(\nu_2 - 1) + n_3(\nu_3 - 1)$.

$$\boxed{N = n_i\nu_i \text{ for } 1 \le i \le t} \tag{2}$$

Since the following argument is quite tedious, the reader may choose to skip to Equation (3) on first reading. This can be done without sacrificing a basic understanding of the development. An argument establishing Equation (2) using the following paragraph and the footnote is presented for those who are already familiar with group theory. The role of Equation (2) is to facilitate the analysis of the implications of Equation (1).

Let i be any positive integer such that $1 \le i \le t$. Then for this particular i we want to show that $N = n_i\nu_i$. Consider the pole points belonging to $\mathsf{C}_i(\mathsf{G})$. For each p_{ij}, there exists at least one rotation $g \in \mathsf{G}$ such that $g(p_{i1}) = p_{ij}$. We single out one such rotation for each j and label it g_j. Then for each $1 \le j \le n_i$, $g_j(p_{i1}) = p_{ij}$. By the way the g_j's were chosen, the collection of pole points $\{g_1(p_{i1}), g_2(p_{i1}), \cdots, g_{n_i}(p_{i1})\} = \{p_{i1}, p_{i2}, \cdots, p_{in_i}\} = \mathsf{C}_i(\mathsf{G})$. We now form the following list where as before, h_{i1} is a generator of H_{i1} (*i.e.*, $\mathsf{H}_{i1} = \{h_{i1}, h_{i1}^2, \cdots, h_{i1}^{\nu_i}\}$):

$$\begin{array}{l} g_1h_{i1}, g_1h_{i1}^2, \cdots, g_1h_{i1}^{\nu_i} \\ g_2h_{i1}, g_2h_{i1}^2, \cdots, g_2h_{i1}^{\nu_i} \\ \vdots \quad\quad \vdots \quad\quad\quad \vdots \\ g_{n_i}h_{i1}, g_{n_i}h_{i1}^2, \cdots, g_{n_i}h_{i1}^{\nu_i}* \end{array}$$

We now wish to show that every rotation in G appears in this listing exactly once so that the number of entries in the list equals $\#(\mathsf{G}) = N$. Let $g \in \mathsf{G}$, then, since g maps p_{i1} to an equivalent pole point, $g(p_{i1}) \in \mathsf{C}_i(\mathsf{G})$ and hence $g(p_{i1}) = p_{ij} = g_j(p_{i1})$ for some $1 \le j \le n_i$. Therefore, $g_j^{-1}g(p_{i1}) = p_{i1}$. Accordingly, $g_j^{-1}g \in \mathsf{H}_{i1} = \{h_{i1}, h_{i1}^2, \cdots, h_{i1}^{\nu_i}\}$ and so $g_j^{-1}g = h_{i1}^k$ for some

* Those familiar with group theory will recognize that each row in our list is actually an enumeration of a coset of H_{i1}. Furthermore, the rotations in G that rotate p_{i1} to p_{ik} are all listed in the k^{th} row. Hence each row corresponds to a pole point in $\mathsf{C}_i(\mathsf{G})$ and conversely. Consequently there is a one-to-one correspondence between the number of pole points in $\mathsf{C}_i(\mathsf{G})$ and cosets of H_{i1}. Hence there are n_i cosets of H_{i1} and since $\#(\mathsf{H}_{ij}) = \nu_i$ we have, by Lagrange's theorem, $N = n_i\nu_i$.

$1 \leq k \leq \nu_i$. Hence, $\boldsymbol{g} = \boldsymbol{g}_r\boldsymbol{h}_{i1}^k$ which appears in our list. Since $\boldsymbol{g}$ is an arbitrarily chosen rotation of G, we may conclude that every rotation in G appears in the list at least once. Our next task is to show that no rotation of G appears more than once in the list. Suppose that $\boldsymbol{g} \in \mathsf{G}$ appears in the list as $\boldsymbol{g} = \boldsymbol{g}_r\boldsymbol{h}_{i1}^k$ and as $\boldsymbol{g} = \boldsymbol{g}_s\boldsymbol{h}_{i1}^m$ with $1 \leq k, m \leq \nu_i$ and $1 \leq r, s \leq n_i$. We wish to show under these circumstances that $r = s$ and $k = m$. Since p_{i1} is a pole point associated with $\boldsymbol{h}_{i1}$, we have $\boldsymbol{g}_r\boldsymbol{h}_{i1}^k(p_{i1}) = \boldsymbol{g}_r(p_{i1}) = p_{ir}$ and $\boldsymbol{g}_s\boldsymbol{h}_{i1}^m(p_{i1}) = \boldsymbol{g}_s(p_{i1}) = p_{is}$. Since $\boldsymbol{g}_r\boldsymbol{h}_{i1}^k = \boldsymbol{g}_s\boldsymbol{h}_{i1}^m$, by the definition of equal mappings, $p_{ir} = p_{is}$ and so $r = s$. With this result we can now write $\boldsymbol{g}_r\boldsymbol{h}_{i1}^k = \boldsymbol{g}_r\boldsymbol{h}_{i1}^m$ which implies by the cancellation law that $\boldsymbol{h}_{i1}^k = \boldsymbol{h}_{i1}^m$ and so $k = m$ since $1 \leq k, m \leq \nu_i$. Therefore, $r = s$ and $k = m$ as required. Thus, we have shown that every rotation in G appears exactly once in the list. Since the list consists of n_i rows and ν_i columns, there are $n_i\nu_i$ symbols listed, and since each rotation in G is listed exactly once, we conclude that $\#(\mathsf{G}) = N = n_i\nu_i$.

Returning to our example group 322, we construct the same list as in the general case using p_{31} as our pole point, and $[110]2$ as the generator of the group H_{31}. Since $1(p_{31}) = p_{31} = [110]2(p_{31})$, $3(p_{31}) = p_{32} = [010]2(p_{31})$, and $3^{-1}(p_{31}) = p_{33} = [100]2(p_{31})$, we must select $\boldsymbol{g}_1$ to be either 1 or $[110]2$, $\boldsymbol{g}_2$ to be either 3 or $[010]2$, and $\boldsymbol{g}_3$ to be either 3^{-1} or $[100]2$. We will choose 1 as $\boldsymbol{g}_1$, 3 as $\boldsymbol{g}_2$, and $[100]2$ as $\boldsymbol{g}_3$. Hence, our list for 322 using p_{31} as our pole point and $[110]2$ as our generator of H_{31} is as follows:

$$\begin{array}{cc} 1^{[110]}2 & 1^{[110]}2^2 \\ 3^{[110]}2, & 3^{[110]}2^2 \\ {[100]}2^{[110]}2, & {[100]}2^{[110]}2^2 \end{array}$$

After forming these compositions (see Table 4), the list becomes

$$\begin{array}{cc} {[110]}2, & 1 \\ {[010]}2, & 3 \\ 3^{-1}, & {[100]}2. \end{array}$$

It is apparent that each rotation of 322 is listed exactly once and that $\nu_3 \cdot n_3 = 2 \cdot 3 = 6 = \#(322)$.

$$\boxed{2 - 2/N = \sum_{i=1}^{t} (1 - 1/\nu_i)} \qquad (3)$$

Since $N = n_i\nu_i$, it follows that $n_i = N/\nu_i$. Replacing n_i in Equation (1) by N/ν_i we obtain

$$2(N - 1) = \sum_{i=1}^{t} (N/\nu_i)(\nu_i - 1)$$

$$2(N - 1) = \sum_{i=1}^{t} N(1 - 1/\nu_i)$$

$$2 - 2/N = \sum_{i=1}^{t} (1 - 1/\nu_i).$$

Because H_{ij} is a subgroup of G, we can conclude that $\#(\mathsf{H}_{ij}) = \nu_i \leq \#(\mathsf{G}) = N$. Also, since H_{ij} is the set of all rotations in G that leave the pole point p_{ij} fixed, it must, by the definition of a pole point, contain at least one rotation in addition to the identity. Hence $2 \leq \nu_i \leq N$. Using the fact that ν_i must be greater than or equal to 2, the right member of Equation (3) satisfies the inequaltiy

$$\sum_{i=1}^{t} (1 - 1/\nu_i) \geq \sum_{i=1}^{t} (1 - 1/2) = \sum_{i=1}^{t} (1/2) = t/2.$$

Also, since $N \geq 2$, we can write

$$2 > 2 - 2/N = \sum_{i=1}^{t} (1 - 1/\nu_i) \geq t/2.$$

Therefore, $2 > t/2$ and hence $4 > t$. Thus t can only be equal to 1, 2, or 3. We can thus conclude that there are no rotation groups having more than 3 equivalence classes of pole points. We now examine each of these three cases for the value of t.

Case where $t = 1$. In this case, Equation (3) becomes

$$2 - 2/N = \sum_{i=1}^{1} (1 - 1/\nu_i) = (1 - 1/\nu_1)$$

$$\text{or} \quad 1 - 2/N = -1/\nu_1.$$

The left member of this equation is always nonnegative because $N \geq 2$, but the right member is always negative because $\nu_1 \geq 2$, which is a contradiction. Therefore, t cannot equal 1, from which we conclude that $\mathcal{P}(\mathsf{G})$ must contain more than one equivalence class of pole points; t must equal 2 or 3.

Case where $t = 2$. In this case Equation (3) becomes

$$2 - 2/N = \sum_{i=1}^{2} (1 - 1/\nu_i)$$

$$= (1 - 1/\nu_1) + (1 - 1/\nu_2)$$

By a little algebraic manipulation we find that

$$2 = N/\nu_1 + N/\nu_2.$$

From Equation (2) we have that $N/\nu_i = n_i$, and so the above expression simplifies to

$$2 = n_1 + n_2 \cdot$$

Because n_1 and n_2 are positive integers, we conclude

TABLE 6. Possible Proper Crystallographic Point Groups

Symbol for $\mathbf{G} = \nu_1\nu_2\nu_3$	$\#(\mathbf{G}) = N$	$\#(\mathbf{C}_1(\mathbf{G})) = N/\nu_1$	$\#(\mathbf{C}_2(\mathbf{G})) = N/\nu_2$	$\#(\mathbf{C}_3(\mathbf{G})) = N/\nu_3$	
222	4	2	2	2	
322	6	2	3	3	
422	8	2	4	4	Dihedral groups
622	12	2	6	6	
332†	12	4	4	6	Tetrahedral group
432	24	6	8	12	Octahedral group

† The group 332 is usually designated by 23.

that $n_1 = n_2 = 1$ is the only possible solution. Hence, for a rotation group with $t = 2$, we have two equivalence classes consisting of one pole point each. Altogether G has a total of two pole points, which accordingly define one and only one rotation axis. Therefore, those groups with two equivalence classes of pole points must be the monaxial groups given in Table 3. The number of elements in each of these possible monaxial groups is equal to the order of the rotation axis, $\#(\mathbf{G}) = \nu_1 = \nu_2$.

Case where $t = 3$. In this case Equation (3) expands to

$$2 - 2/N = (1 - 1/\nu_1) + (1 - 1/\nu_2) + (1 - 1/\nu_3)\cdot$$

Rewriting this result we see that

$$1 + 2/N = 1/\nu_1 + 1/\nu_2 + 1/\nu_3 \cdot \qquad (4)$$

Since $N \geq 2$, it follows that $1 + 2/N > 1$ and so

$$1/\nu_1 + 1/\nu_2 + 1/\nu_3 > 1 \cdot \qquad (5)$$

For convenience, we can assume that $\nu_1 \geq \nu_2 \geq \nu_3$.

In constructing Table 6 we have considered all possible combinations of ν_1, ν_2, and ν_3; selected from the permissible values 2, 3, 4, and 6; and recorded those that satisfy Inequality (5). Note that the other possibilities for $\nu_1\nu_2\nu_3$ are 632, 442, 642, 662, 333, 433, 633, 443, 643, 663, 444, 644, 664, and 666. A quick check shows that none of these sets satisfy Inequality (5). (Note that the derivation of Inequality (5) did not require ν_1, ν_2, and ν_3 to be 2, 3, 4, or 6. Hence a large number non-crystallographic point groups may be formed that satisfy Inequality (5). For example, $n22$ satisfies (5) for all $n > 1$.) * The orders of each of the potential polyaxial crystallographic point groups in Table 6 are found by substituting ν_1, ν_2, and ν_3 into Equation (4) and solving to obtain $N = \#(\mathbf{G}) = 2\nu_1\nu_2\nu_3/(\nu_1\nu_2 + \nu_2\nu_3 + \nu_3\nu_1 - \nu_1\nu_2\nu_3)$. The order of $\mathbf{C}_i(\mathbf{G}) = n_i$ is found by appealing to Equation (2), which yields $n_i = N/\nu_i$. These are also recorded in Table 6.

Determination of the interaxial angles

We have shown above that there are only 11 possible proper crystallographic point groups, namely 1, 2, 3, 4, 6, 222, 322, 422, 622, 332, and 432. The monaxial groups 1, 2, 3, 4, and 6 were established earlier. However, we have not yet established the fact that each of the polyaxial combinations actually yields a group. Also, the possibility remains that some of these combinations may lead to two or more groups which may arise by assuming different intersection angles between the rotation axes (these angles are called interaxial angles.). We will see later in this section, however, that each of the possibilities leads to precisely one point group. In the process we will actually determine the interaxial angles used in the formation of these point groups. Inherent in the strategy we will follow in determining these interaxial angles is the observation that before a polyaxial combination qualifies as a group it must satisfy the requirement that each of its rotations permutes the pole points within each of the three equivalence classes. Hence a rotation must map a given pole point to another pole point in the same equivalence class. We recall that because equivalence classes are disjoint no two distinct equivalence classes share a common pole point. This observation will also be of considerable use in the determination of the interaxial angles. In addition it will be helpful to observe that if a half-turn maps the point $p \in \mathcal{S}$ to q then its axis must bisect both of the arcs determined by p and q. Hence, if r is a pole point of such a half-turn, then $\widehat{pr} = \widehat{qr}$.

Interaxial angles for the dihedral groups $\nu_1 22$

We begin by considering the interaxial angles that must exist for a polyaxial combination of the form

* See Klein, Weyl, or Zassenhaus for a derivation of the non-crystallographic rotation groups based on these ideas.

$\nu_1 22$ (when $\nu_1 = 2, 3, 4, 6$) to be a group. Table 6 shows that there are exactly two pole points which we denote p_{11} and p_{12} in the equivalence class $C_1(\nu_1 22)$. Let $\boldsymbol{h}$ be a non-identity rotation in G such that $\boldsymbol{h}(p_{11}) = p_{11}$, *i.e.*, $\boldsymbol{h} \in H_{11}$. Then $\boldsymbol{h}(p_{12})$ must equal p_{11} or p_{12} since every rotation in $\nu_1 22$ must permute the equivalence class $C_1(\nu_1 22) = \{p_{11}, p_{12}\}$. Because it was assumed above that $\boldsymbol{h}(p_{11}) = p_{11}$ and because $\boldsymbol{h}$ cannot map two distinct pole points to the same pole point, we conclude that $\boldsymbol{h}(p_{12})$ must not equal p_{11} and hence $\boldsymbol{h}(p_{12}) = p_{12}$. Therefore p_{11} and p_{12} both lie on the axis of the rotation $\boldsymbol{h}$. Consequently, p_{11} and p_{12} are antipodal points and so there is exactly one ν_1-fold axis associated with $C_1(\nu_1 22)$. Also each of the equivalence classes associated with the cyclic groups of order 2 contain ν_1 pole points. Accordingly, we write $C_2(\nu_1 22) = \{p_{21}, p_{22}, \cdots, p_{2\nu_1}\}$ and $C_3(\nu_1 22) = \{p_{31}, p_{32}, \cdots, p_{3\nu_1}\}$. Moreover, since there is a total of $\#(C_2(\nu_1 22)) + \#(C_3(\nu_1 22)) = 2\nu_1$ pole points associated with the 2-fold axes, there must be exactly ν_1 2-fold axes associated with $C_2(\nu_1 22)$ and $C_3(\nu_1 22)$. Now that we know the number of each kind of rotation axis present in $\nu_1 22$, the task is to discover the appropriate interaxial angles between these axes so as to form a group. If we place the Z axis along the ν_1-fold axis, then p_{11} and p_{12} are the points where the Z axis intersects with the surface S of the unit sphere. The question now is "Where can a 2-fold axis associated with say p_{21} be placed so that the associated half-turn $\boldsymbol{g}$ will permute $\{p_{11}, p_{12}\}$?" If $\boldsymbol{g}(p_{11}) = p_{11}$, then $\boldsymbol{g}(p_{12}) = p_{12}$. Since $\boldsymbol{g}$ has only two pole points, p_{21} must be either p_{11} or p_{12}, which is a contradiction because the equivalence classes of pole points are disjoint. Hence $\boldsymbol{g}(p_{11}) = p_{12}$, and p_{21} bisects the arc $\overset{\frown}{p_{11}p_{12}}$. Therefore, since $\overset{\frown}{p_{11}p_{21}} = \overset{\frown}{p_{21}p_{12}}$ and since $\overset{\frown}{p_{11}p_{21}} + \overset{\frown}{p_{21}p_{12}} = 180°$, it follows that $\overset{\frown}{p_{11}p_{21}} = 90°$. Accordingly, it follows that the 2-fold axis associated with p_{21} must be perpendicular to the ν_1-fold axis. A similar argument shows that the 2-fold axes associated with the remaining pole points in $C_2(\nu_1 22)$ and $C_3(\nu_1 22)$ are also perpendicular to the ν_1-fold axis. Thus, the ν_1 2-fold axes in $\nu_1 22$ are all perpendicular to the ν_1-fold axis.

The remaining question is "What must the interaxial angles be between these 2-fold axes?" Without loss of generality, because p_{21} is on the equator (the great circle perpendicular to Z), we can place the X axis of our coordinate system so that it passes through p_{21}. We know that the images of p_{21} under the rotations along the ν_1-fold axis are all in $C_2(\nu_1 22)$. Moreover, because of the nature of the rotations about the ν_1-fold axis, we obtain ν_1 points (hence all of the points in $C_2(\nu_1 22)$) spaced equally on the equator so that the arc length between any two adjacent points is $360°/\nu_1$.

We now observe that there is only one rotation $\boldsymbol{h}$ associated with the pole points in $C_1(\nu_1 22)$ such that $\boldsymbol{h}(p_{21}) = p_{22}$ where p_{21} and p_{22} are adjacent pole points in $C_2(\nu_1 22)$. If we let $^{[100]}\boldsymbol{2}$ denote the half-turn about the X axis then $^{[100]}\boldsymbol{2}(p_{21}) = p_{21}$, and the rotation $\boldsymbol{h}^{[100]}\boldsymbol{2}$ has the property that $\boldsymbol{h}^{[100]}\boldsymbol{2}(p_{21}) = p_{22}$. However, $\boldsymbol{h}^{[100]}\boldsymbol{2} \neq \boldsymbol{h}$ because if $\boldsymbol{h}^{[100]}\boldsymbol{2} = \boldsymbol{h}$, then $\boldsymbol{h}^{[100]}\boldsymbol{2} = \boldsymbol{h} \cdot \boldsymbol{1}$ which according to the cancellation law would yield the contradiction that $^{[100]}\boldsymbol{2} = \boldsymbol{1}$. But $\boldsymbol{h}$ was the only rotation associated with $C_1(\nu_1 22)$ which maps p_{21} to p_{22}. Hence $\boldsymbol{h}^{[100]}\boldsymbol{2}$ must be a rotation associated with a pole point in either $C_2(\nu_1 22)$ or $C_3(\nu_1 22)$. Therefore $\boldsymbol{h}^{[100]}\boldsymbol{2}$ must be a half-turn which maps p_{21} to p_{22} and whose rotation axis is perpendicular to the Z axis. Thus the axis of $\boldsymbol{h}^{[100]}\boldsymbol{2}$ must bisect the arcs along the equator determined by p_{21} and p_{22}. Let q denote the pole point belonging to $\boldsymbol{h}^{[100]}\boldsymbol{2}$ which bisects the shorter arc between p_{21} and p_{22}. Since p_{21} and p_{22} are adjacent pole points in $C_2(\nu_1 22)$, q cannot be in $C_2(\nu_1 22)$ and hence must be in $C_3(\nu_1 22)$. The images of q under the rotations about the ν_1-fold axis are the remaining pole points in $C_3(\nu_1 22)$. In summary, we have shown that, if $\nu_1 22$ (where $\nu_1 = 2, 3, 4, 6$) is to be a group, there is only one possible arrangement of rotation axes. The interaxial angles for this arrangement are such that the angle between the ν_1-fold rotation axis and each of the 2-fold rotation axes associated with the pole points in $C_2(\nu_1 22)$ and $C_3(\nu_1 22)$ is 90° and the angle between any two adjacent 2-fold axes is $180°/\nu_1$. Referring to Figure 4, we see that our example group 322 does indeed satisfy this interaxial criteria. The fact that $\nu_1 22$ actually forms a group when its interaxial angles are as described above can be shown by preparing a multiplication table (note that this can now be easily done by those familiar with matrix theory since the matrix representation for the rotations in $\nu_1 22$ is completely determined by the interaxial angles).

Interaxial angles for the tetrahedral group 332 *(i.e.,* 23*)*

Our next task is to determine the interaxial angles for 332. It is clear from Table 6 that there are two equivalence classes associated with the 3-fold axes containing 4 points each, and one equivalence class of pole points associated with the 2-fold axes containing 6 pole points. Accordingly, there are four 3-fold axes and three 2-fold axes in 332.

We begin by considering the placement of the three 2-fold axes. Let p_{31} denote a point in $C_3(332)$. Since

$C_3(332)$ contains all of the pole points associated with the half-turns in G and since the antipodal point of p_{31} is associated with the same half-turn associated with p_{31}, it follows that the antipodal point of p_{31}, which we denote by p_{32}, is in $C_3(332)$. Without loss of generality, we place the Z axis along the line segment $\overline{p_{31}p_{32}}$. Let p_{33} be any one of the remaining pole points in $C_3(332)$. We will show that $\widehat{p_{31}p_{33}} = 90°$ by assuming that $\widehat{p_{31}p_{33}} \neq 90°$ and arriving at a contradiction. If $\widehat{p_{31}p_{33}} \neq 90°$, then either $\widehat{p_{31}p_{33}} < 90°$ or $\widehat{p_{31}p_{34}} < 90°$ where p_{34} is antipodal to p_{33}. Without loss of generality, we may assume that $\widehat{p_{31}p_{33}} < 90°$. If we let 2 denote the half-turn along the Z axis (with pole points p_{31},p_{32}), then $2(p_{33}) = p_{3j}$ for some $p_{3j} \in C_3(332)$. Hence $\widehat{p_{31}p_{3j}} = \widehat{p_{31}p_{33}} < 90°$. By our earlier observation on the effect of a half-turn, p_{31} bisects $\widehat{p_{3j}p_{33}}$, hence $\widehat{p_{3j}p_{33}} < 90° + 90° = 180°$. Therefore $p_{3j} \neq p_{34}$ since $\widehat{p_{34}p_{33}} = 180°$. Moreover, it is clear that $p_{3j} \notin \{p_{31},p_{32},p_{33}\}$. Hence the rotation axis associated with p_{3j} is different from those associated with $\{p_{31},p_{32}\}$ and $\{p_{33},p_{34}\}$. Therefore, p_{3j} must be one of the remaining pole points in $C_3(332)$, say $p_{3j} = p_{35}$. We also observe, since p_{31} bisects $\widehat{p_{35}p_{33}}$, that $\overrightarrow{Op}_{31}$, $\overrightarrow{Op}_{33}$ and $\overrightarrow{Op}_{35}$ are coplanar where $\overrightarrow{O}$ is the origin of R^3. Hence the three axes associated with half-turns are all coplanar. We now make an obvious but important observation about third-turns. If $\boldsymbol{g}$ is a third-turn and q is a point not on its rotation axis, then the points $\{q,\boldsymbol{g}(q),\boldsymbol{g}^2(q)\}$ determine a plane perpendicular to the axis of $\boldsymbol{g}$. Hence given any point q in $C_3(332)$ and any 3-fold axis belonging to 332, there exist two other pole points in $C_3(332)$ such that the plane determined by q and these other two points is perpendicular to the 3-fold axis. But, under the hypothesis that $\widehat{p_{31}p_{33}} \neq 90°$, we have shown that all the pole points of $C_3(332)$ are coplanar and hence all of the 3-fold axes must be perpendicular to the plane determined by these pole points. This means that 332 can have only one 3-fold axis, which is a contradiction because we know that there are four such axes. Therefore, the angle $\widehat{p_{31}p_{33}} = 90°$. Since p_{31} was an arbitrarily chosen point in $C_3(332)$ and since p_{33} was selected to be any pole point except p_{31} and p_{32}, we see by similar reasoning that $\widehat{p_{31}p_{35}} = 90°$ and $\widehat{p_{33}p_{35}} = 90°$. Consequently, the three 2-fold axes are mutually perpendicular. Note that this says that 222 is contained in 332.

Now we will turn to the placement of the four 3-fold axes. Let p_{11} be a pole point in $C_1(332)$. Then p_{11} appears on S in one of the octants delineated by the three 2-fold axes. Without loss of generality, we can assume that p_{11} is located somewhere in the first octant (denoted by the shaded region in Fig. 5). If we let p_{31} play the role of q in our observation in the previous paragraph, then we know that the 3-fold axis through p_{11} is perpendicular to some plane containing p_{31} and two other pole points in $C_3(332)$. By inspecting all such planes containing p_{31} and remembering that the 3-fold axis cannot be coincident with any of the 2-fold axes, it is clear that the plane determined by p_{31}, p_{33}, and p_{35} (see Fig. 5) is the only possibility. Therefore the third-turn associated with p_{11} maps p_{31} to p_{33}, p_{33} to p_{35}, and p_{35} to p_{31} requiring that p_{11} be equidistant from the points p_{31}, p_{33}, and p_{35} (see Fig. 6a). Therefore $\widehat{p_{31}p_{11}} = \widehat{p_{33}p_{11}} = \widehat{p_{35}p_{11}}$. Solving in the standard way the spherical triangles that arise from these relationships, we conclude that $\widehat{p_{31}p_{11}} = 54.74°$. The images of p_{11} under the half-turns in 332 yield the four pole points belonging to $C_1(332) = \{p_{11}, p_{12}, p_{13}, p_{14}\}$ as pictured in Figure 6a. The antipodal points to those appearing in $C_1(332)$ are not in $C_1(332)$, but they are the pole points that form $C_2(332)$. The resulting set of all pole points belonging to 332 are shown in Figure 6b. We have therefore shown that this arrangement yields the only possibility for 332 to be a group. If a multiplication table is prepared, it can be shown that this arrangement does indeed yield a group. A list of selected interaxial angles between the rotation axes in 332 is given in Figure 6c, from which the remaining angles may be deduced.

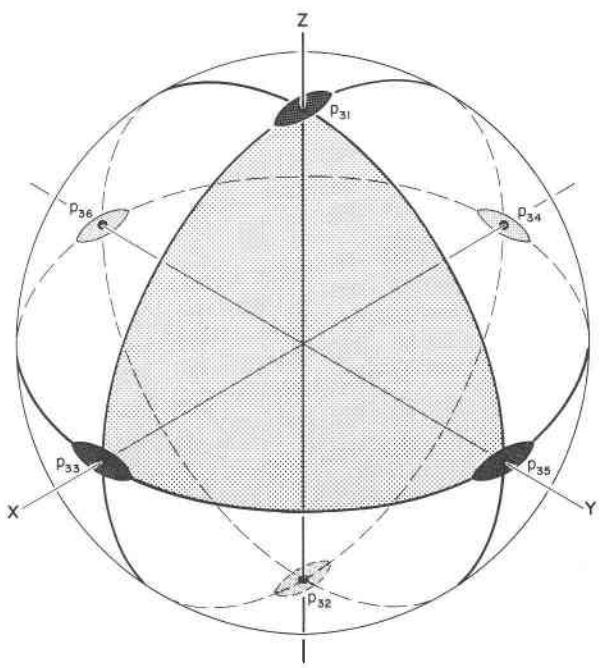

FIG. 5. The orientations of the 2-fold rotation axes for the tetrahedral group 332 ≡ 23 with their associated pole points shown as solid circles. The surface area on the unit sphere where pole point p_{11} must lie is shaded.

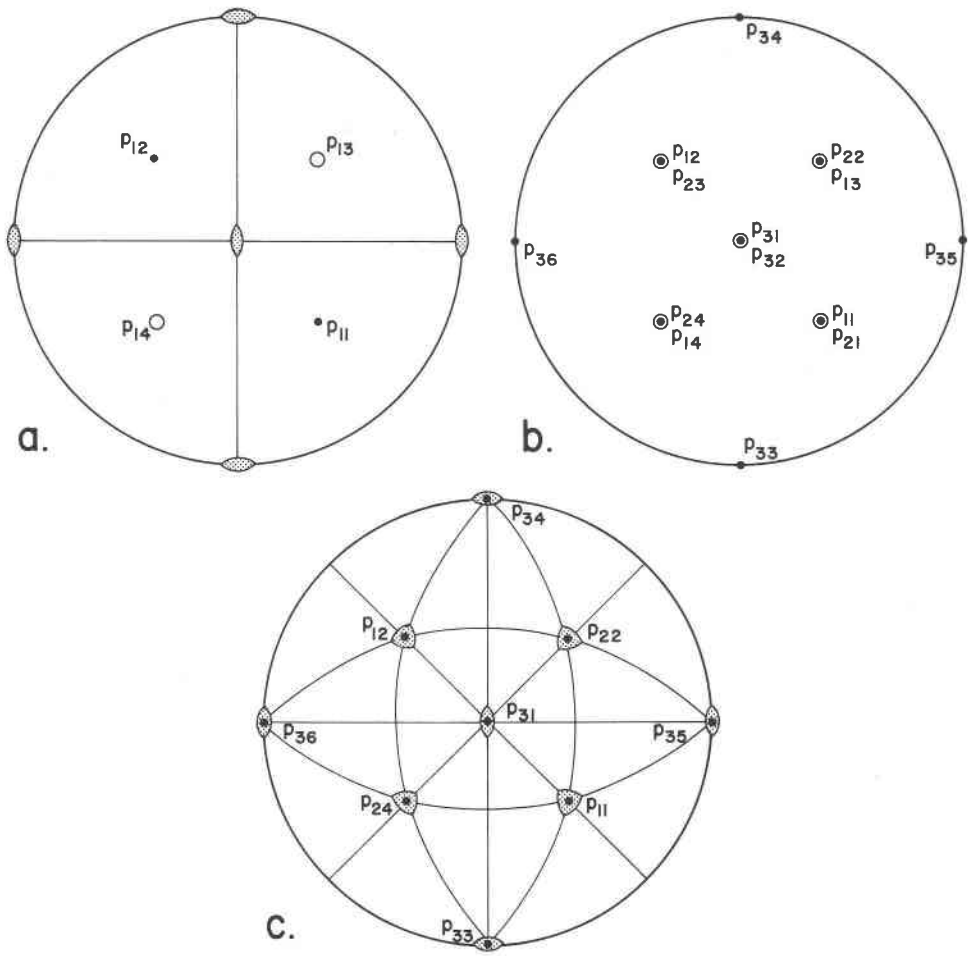

FIG. 6. (a.) Stereographic projection of the 2-fold rotation axes of the tetrahedral group and the pole points belonging to $C_1(332)$ where the solid circles denote points on the upper hemisphere and the open circles denote points on the lower hemisphere. (b.) Stereographic projection of all the pole points for the tetrahedral group. (c.) Stereographic projection of the rotation axes of the tetrahedral group and pole points appearing in the upper hemisphere. Selected interaxial angles are given by the following arc lengths: $\widehat{p_{31}p_{11}} = \widehat{p_{11}p_{33}} = \widehat{p_{11}p_{35}} = \widehat{p_{31}p_{22}} = \widehat{p_{31}p_{12}} = \widehat{p_{31}p_{24}} = 54.74°$; $\widehat{p_{11}p_{22}} = \widehat{p_{22}p_{12}} = \widehat{p_{12}p_{24}} = \widehat{p_{24}p_{11}} = 70.32°$; $\widehat{p_{11}p_{12}} = \widehat{p_{22}p_{24}} = 109.47°$; $\widehat{p_{31}p_{34}} = 90°$; $\widehat{p_{11}p_{34}} = 125.26°$.

Interaxial angles for the octahedral group 432

The final case in our consideration of proper rotation groups is 432, which has three 4-fold axes, four 3-fold axes, and six 2-fold axes (see Table 6). Implicit in the three 4-fold axes are three 2-fold axes. Since there are more than one 3-fold axes present, the argument given in our discussion of 332 allows us to conclude that the three 4-fold axes are mutually perpendicular. We use the same orientation for these 4-fold axes as for the 2-fold axes in 332 (see Fig. 5). Since the 6 pole points belonging to the 4-fold axes in 432 are arranged in exactly the same way as the 6 pole points belonging to the 2-fold axes in 332, the 3-fold axes in 432 must also be arranged in the same manner. That is to say that 332 is contained in 432. Hence we have placed all of the 4-fold and 3-fold axes present in 432 (see Fig. 7a). Since there are half-turns implicit in the horizontally placed 4-folds and since these axes are perpendicular to the vertically placed four-fold axis, we can conclude that 422 is contained in 432. Hence by our discussion of 422 we know that there are 2-fold axes bisecting the horizontal 4-fold axes. Hence the point p_{31} placed as shown in Figure 7a is a pole point belonging to $C_3(432)$. The remaining eleven pole points in $C_3(432)$ can be found by locating the images of p_{31} under the rotations of 432 which have already been placed. The placement

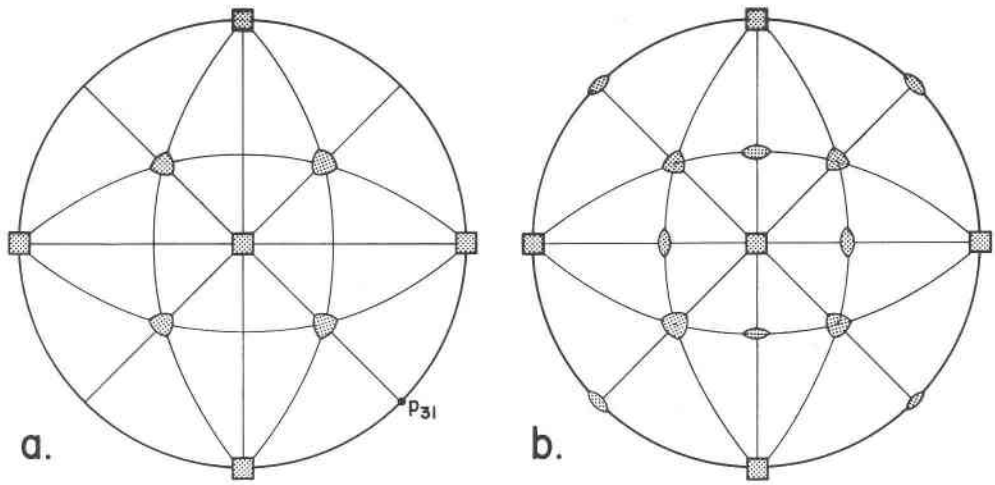

FIG. 7. (a.) Stereographic projection of the 3-fold and 4-fold rotation axes and pole point p_{31} for the octahedral group 432. (b.) Stereographic projection of the rotation axes for the octahedral group.

of all the rotations of group 432 are shown in Figure 7b. The interaxial angles can be deduced from those given for 332. Also we note that by forming a multiplication table, one can verify that this arrangement of the axes involved in 432 does in fact yield a group.

In summary we have found interaxial angles for the eleven proper crystallographic point groups 1, 2, 3, 4, 6, 222, 322, 422, 622, 332, and 432. It can be shown that for each of these groups there exists a lattice that is left invariant under each of the rotations of the group and so they are all *bonafide* crystallographic point groups (Boisen and Gibbs, in preparation). Furthermore, we have shown that there are no other proper crystallographic point groups.

Improper crystallographic point groups

In the previous section we showed that there are only 11 proper rotation groups, and we derived each of them. In this section we will show how each of the improper crystallographic point groups can be constructed from these proper crystallographic point groups. This will be easily accomplished once we have established the following important theorem.

Theorem 2. If I is an improper crystallographic point group, then there exists a proper crystallographic point group G such that either

(1) $\mathsf{I} = \mathsf{G} \cup \mathsf{G}i$ where i is the inversion. (Here $\mathsf{G}i = \{gi | g \in \mathsf{G}\}$)

or

(2) $\mathsf{I} = \mathsf{H} \cup (\mathsf{G}\backslash\mathsf{H})i$ where H is a subgroup of G such that $\#(\mathsf{G})/\#(\mathsf{H}) = 2$. (Here $(\mathsf{G}\backslash\mathsf{H})i = \{gi | g \in \mathsf{G}$ and $g \notin \mathsf{H}\}$)

Furthermore, all of the sets constructed from a proper crystallographic group G as in (1) or (2) are groups and hence improper crystallographic point groups.

Before presenting the proof of Theorem 2 we will use the theorem to derive the collection of all improper crystallographic point groups, give some examples, and record in Table 7 all of the crystallographic point groups.

If H is a subgroup of G such that $\#(\mathsf{G})/\#(\mathsf{H}) = 2$, then we say that H is a *halving group*. This theorem shows that if we take each proper crystallographic point group G one at a time and first form $\mathsf{G} \cup \mathsf{G}i$ and then $\mathsf{H} \cup (\mathsf{G}\backslash\mathsf{H})i$ for each of its halving groups H (note that in certain cases G does not have any halving groups), then the resulting collection of groups is precisely the collection of all improper crystallographic point groups.

Note that the improper crystallographic point groups of the form $\mathsf{G} \cup \mathsf{G}i$ have order $2\#(\mathsf{G})$ and are those that contain the inversion (since $1 \in \mathsf{G}$). Hence we have a total of eleven improper rotation groups that contain the inversion. When a group G has a halving group H, then we can form the improper crystallographic group $\mathsf{H} \cup (\mathsf{G}\backslash\mathsf{H})i$ which has order $\#(\mathsf{G})$ and has the property that it does not contain the inversion (since $1 \notin (\mathsf{G}\backslash\mathsf{H})$). Table 7 shows that there are ten such groups, bringing the total number of crystallographic point groups to 32.

If Φ is a rotoinversion such that $\Phi \in \mathsf{G} \cup \mathsf{G}i$ or $\Phi \in \mathsf{H} \cup (\mathsf{G}\backslash\mathsf{H})i$, then there exists an element $g \in \mathsf{G}$ such that $\Phi = gi$. By the definition of the rotation axis of an improper rotation given earlier,

TABLE 7. The 32 Crystallographic Point Groups and Their Orders as Derived From the Proper Crystallographic Point Groups

The 11 Proper Crystallographic Point Groups		Halving Groups*	The 21 Improper Crystallographic Point Groups			
			Containing i (centrosymmetrical)		Not containing i	
G	#(G)	H	G ∪ Gi	#(G ∪ Gi)	H ∪ (G\H)i	#(H ∪ (G\H)i)
1	1	none	$\bar{1}$	2	none	—
2	2	1	$2/m$	4	m	2
3	3	none	$\bar{3}$	6	none	—
4	4	2	$4/m$	8	$\bar{4}$	4
6	6	3	$6/m$	12	$\bar{6}$	6
222	4	2	mmm	8	$mm2$	4
322	6	3	$\bar{3}2/m$	12	$3mm$	6
422	8	4	$4/mmm$	16	$4mm$	8
		222			$\bar{4}2m$	8
622	12	6	$6/mmm$	24	$6mm$	12
		322			$\bar{6}2m$	12
332 = 23	12	none	$2/m\bar{3}$	24	none	—
432	24	23	$4/m32/m$	48	$\bar{4}3m$	24

* The halving groups H of a given proper crystallographic point group G can be easily found by examining those groups in column 1 that have one half the number of elements as G. If L is in column 1 such that # (L) = # (G)/2, then L is a halving group of G if (1) all of the rotations of L also appear in G and (2) the corresponding interaxial angles between these rotations are the same in L as in G. In certain cases like 422 where 222 occurs in more than one orientation, there is technically more than one group of the form H ∪ (G\H)i for a given H. However, the construction of these groups results in the same point group but in different orientations, and consequently we do not make a distinction between them.

the rotation axis of Φ is the same as that of $\boldsymbol{g}$. Hence, the rotation axes appearing in G ∪ Gi and H ∪ (G\H)i are the same as those in G Therefore it follows that the interaxial angles obtained for G apply to both G ∪ Gi and H ∪ (G\H)i as well. By the way Table 7 is constructed and because of the relationship between the proper and improper groups, all the crystallographic point groups with the same interaxial angles appear in the same row. We note again that in this paper we have not demonstrated for each of these crystallographic groups the existence of a lattice Γ which is left invariant. However, this fact can be shown and will be explored in a future paper.

We will now do several examples of the construction described in Theorem 2 followed by Table 7 showing the results we obtain by applying this construction to all eleven proper crystallographic point groups. We recall that the orientation symbo attached to a given rotation or rotoinversion is dependent on the choice of the basis. In each of our examples the basis will be chosen to be consistent with the *International Tables for X-ray Crystallography* (see Table 2.3.1 , Henry and Lonsdale, 1952). We then conclude the paper with the proof of Theorem 2.

To illustrate the use of Theorem 2 in the construction of the improper crystallographic groups, we will first consider the constructions G ∪ Gi and H ∪ (G\H)i where G is the proper monaxial group 6. For this case G ∪ Gi becomes $6 \cup 6i = \{1, 6, 3, 2, 3^{-1}, 6^{-1}\} \cup \{1, 6, 3, 2, 3^{-1}, 6^{-1}\}i = \{1, 6, 3, 2, 3^{-1}, 6^{-1}\} \cup \{1i, 6i, 3i, 2i, 3^{-1}i, 6^{-1}i\} = \{1, 6, 3\ 3^{-1}, 6^{-1}, i, \bar{6}, \bar{3}, m, \bar{3}^{-1}, \bar{6}^{-1}\}$ which is denoted by $6/m$. To construct the group H ∪ (G\H)i, G must contain a subgroup H such that #(H) = #(G)/2. As noted in Table 7, if such an H exists, it must appear in column 1 of the table. In the case under consideration #(6) = 6, hence #(H) = 3. The only group in column 1 with order 3 that qualifies as a possible halving group in 6 is the proper monaxial group 3. Since all the rotations in 3 are contained in 6, we conclude that 3 is the only halving group in 6. Accordingly, it is clear that H ∪ (G\H)i becomes $3 \cup (6\backslash 3)i = \{1, 3, 3^{-1}\} \cup \{6, 2, 6^{-1}\}i = \{1, 3, 3^{-1}, 6i, 2i, 6^{-1}i\} = \{1, 3, 3^{-1}, \bar{6}, m, \bar{6}^{-1}\}$ denoted by $\bar{6}$.

In our next illustration, we will construct G ∪ Gi and H ∪ (G\H)i where G is the proper polyaxial group 322. In this case G ∪ Gi becomes $(322) \cup (322)i = \{1, 3, 3^{-1}, {}^{[100]}2, {}^{[110]}2, {}^{[010]}2, i, \bar{3}, \bar{3}^{-1}, {}^{[100]}m, {}^{[110]}m, {}^{[010]}m\}$ denoted by $\bar{3}2/m$. The monaxial group

3 qualifies as the only halving group in 322 because $\#(3) = 3$ and because all the rotations in 3 are contained in 322. Thus, $\mathsf{H} \cup (\mathsf{G}\backslash\mathsf{H})i$ becomes $3 \cup ((322)\backslash 3)i = \{1, 3, 3^{-1}, [100]m, [110]m, [010]m\}$ denoted by $3mm$.

Finally we consider the improper crystallographic point groups that are constructed from $\mathsf{G} = 422$. The $\mathsf{G} \cup \mathsf{G}i$ is constructed as before and results in the group 4/mmm. Two proper groups 4 and 222 in Table 7 qualify as halving groups in 422. Letting $\mathsf{H} = 4$, we construct $4 \cup ((422)\backslash 4)i = \{1, 4, 2, 4^{-1}, [100]m, [110]m, [010]m, [\bar{1}10]m\}$ denoted by $4mm$. Letting $\mathsf{H} = 222$, we construct $(222) \cup ((422)\backslash(222))i = \{1, 2, [100]2, [010]2, \bar{4}, \bar{4}^{-1}, [110]m, [\bar{1}10]m\}$ denoted by $\bar{4}2m$.

Note that group 332 lacks halving groups despite the fact that groups 322 and 6 both have orders one-half that of 332. This is because a six-fold axis is not contained in 332 and the interaxial angles between the 2-fold and the 3-fold rotation axes in 322 and 332 are different.

Proof of Theorem 2

Let I denote an improper crystallographic point group and let $k_1, k_2, \cdots, k_n$ be the proper rotations in I. We know that I does have some proper rotations since $1 \in \mathsf{I}$, which is a proper rotation. We now consider two cases; (1) $i \in \mathsf{I}$ and (2) $i \notin \mathsf{I}$.

Case where $i \in \mathsf{I}$. In this case, each of isometries $k_1, k_2, \cdots, k_n, k_1i, k_2i, \cdots, k_ni$ are in I. We will show that this is a complete listing of the elements of I. Let $t \in \mathsf{I}$, then we want to show that t appears in the list. If t is a proper rotation, then t already appears in the list $k_1, k_2, \cdots, k_n$. If t is not a proper rotation, then it must be an improper rotation and hence can be written $t = fi$ where f is a proper rotation. Since $i \in \mathsf{I}$ we know that $(fi)i = f \in \mathsf{I}$. Hence $f = k_j$ for some $1 \leq j \leq n$ and consequently $fi = k_ji$ is in the list. Therefore $\mathsf{I} = \{k_1, k_2, \cdots, k_n, k_1i, k_2i, \cdots, k_ni\}$. Since the composition of two proper rotations is again a proper rotation, we see that $\{k_1, k_2, \cdots, k_n\}$ forms a subgroup of I. Let G denote the group consisting of $\{k_1, \cdots, k_n\}$. Then $\mathsf{I} = \mathsf{G} \cup \mathsf{G}i$ and so I is of the form described in statement (1) of the theorem.

Case where $i \notin \mathsf{I}$: Again let $k_1, \cdots, k_n$ denote the proper rotations in I. The set of all improper rotations in I can be written in the form $\{s_1i, s_2i, \cdots s_mi\}$ where s_j is a proper rotation for all $1 \leq j \leq m$. Since $i \notin \mathsf{I}$, s_j is not the identity for all $1 \leq j \leq m$. First we want to show that $m = n$. That is, the number of proper rotations in I equals the number of improper rotations in I. We begin by considering the set of rotations $\{k_1s_1i, k_2s_1i, \cdots, k_ns_1i\}$. By the cancellation law we know that these are distinct rotations. Hence we have found a list of n improper rotations in I. Therefore $n \leq m$. Now consider the set of rotations $\{(s_1i)(s_1i), (s_1i)(s_2i), \cdots, (s_1i)(s_mi)\}$. Since the inversion commutes with any proper rotation we have $(s_1i)(s_ji) = (s_1i)(is_j) = s_1i^2s_j = s_1s_j$ which is a proper rotation. Hence we have that $\{s_1^2, s_1s_2, \cdots, s_1s_m\}$ is a set of m distinct (by the cancellation law) proper rotations in I and so $m \leq n$. Hence $m = n$. Next we consider the set of proper rotations $\mathsf{G} = \{k_1, \cdots, k_n, s_1, \cdots, s_n\}$ (remember that the s_j's are not in I). We will show that G is a group by showing closure. Let $a, b \in \mathsf{G}$. Then we have four cases to consider. First, if a and b are both k's then since they are proper rotations belonging to I, the composition ab is also a proper rotation in I and so ab is one of the k's listed in G. Second, if $a = k_j$ for some $1 \leq j \leq n$ and $b = s_r$ for some $1 \leq r \leq n$, then $ab = k_js_r$. But since $(k_js_r)i = k_j(s_ri) \in \mathsf{I}$, $ab = k_js_r$ is, by the cancellation law, some s_t listed in G. Third, if $a = s_j$ for some $1 \leq j \leq n$ and $b = k_r$ for some $1 \leq r \leq n$, then $ab = s_jk_r$. Since $(s_ji)k_r = s_jk_ri \in \mathsf{I}$, $ab = s_jk_r$ is some s_t listed in G. Fourth, if $a = s_j$ for some $1 \leq j \leq n$ and $b = s_r$ for some $1 \leq r \leq n$, then $ab = s_js_r = s_js_ri^2 = (s_ji)(s_ri) \in \mathsf{I}$. Hence ab is a proper rotation in I and so appears as one of the k's. Therefore it has been shown that G is closed under composition and hence a group. Note that if we set $\mathsf{H} = \{k_1, \cdots, k_n\}$, then H, being the set of all proper rotations in I, is a group and so H is a subgroup of G. Also $\#(\mathsf{G})/\#(\mathsf{H}) = 2n/n = 2$. Since $\mathsf{I} = \{k_1, \cdots, k_n, s_1i, \cdots, s_ni\}$, $\mathsf{I} = \mathsf{H} \cup (\mathsf{G}\backslash\mathsf{H})i$ as required.

Now to establish the final remark of the theorem suppose that G is a proper rotation group. Then, using the techniques employed in the above proof, it is easy to show that $\mathsf{G} \cup \mathsf{G}i$ is closed and hence a group. Next we suppose that G has a subgroup H such that $\#(\mathsf{G})/\#(\mathsf{H}) = 2$. We wish to show that the set $\mathsf{H} \cup (\mathsf{G}\backslash\mathsf{H})i$ is closed and hence a group.* Let $a, b \in \mathsf{H} \cup (\mathsf{G}\backslash\mathsf{H})i$. If $a, b \in \mathsf{H}$ then clearly $ab \in \mathsf{H}$ and so $ab \in \mathsf{H} \cup (\mathsf{G}\backslash\mathsf{H})i$ as required. If $a \in \mathsf{H}$ and $b \in (\mathsf{G}\backslash\mathsf{H})i$, then $b = gi$ for some $g \in \mathsf{G}\backslash\mathsf{H}$. Now $ag \notin \mathsf{H}$ for if $ag \in \mathsf{H}$, then $g = a^{-1}(ag) \in \mathsf{H}$ which is not the case. Hence $ag \in \mathsf{G}\backslash\mathsf{H}$ and so $ab = (ag)i \in (\mathsf{G}\backslash\mathsf{H})i$ and so again $ab \in \mathsf{H} \cup (\mathsf{G}\backslash\mathsf{H})i$. Similarly, if $a \in (\mathsf{G}\backslash\mathsf{H})i$ and $b \in \mathsf{H}$, then $ab \in \mathsf{H} \cup (\mathsf{G}\backslash\mathsf{H})i$. Now suppose that $a, b \in (\mathsf{G}\backslash\mathsf{H})i$. Then $a = g_1i$ and $b = g_2i$ for some $g_1, g_2 \in \mathsf{G}\backslash\mathsf{H}$ and $ab = (g_1i)(g_2i) = g_1g_2$. Hence we want to show that $g_1g_2 \in \mathsf{H}$. We have

* The reader who is familiar with factor groups may recognize immediately that $\mathsf{H} \cup (\mathsf{G}\backslash\mathsf{H})i$ is closed.

proved above that the product of a rotation in (G\H) with a rotation in H is in G\H. Hence $g_1H = \{g_1h \mid h \in H\} \subseteq G\backslash H$. By the cancellation law, $\#(g_1H) = \#(H)$ and so $\#(g_1H) = \#(G\backslash H)$. Therefore $g_1H = G\backslash H$. Consequently, if $g_1g_2 \in G\backslash H$, then $g_1g_2 = g_1h$ for some $h \in H$. But then, by the cancellation law, $g_2 = h \in H$, which is a contradiction. Therefore, $g_1g_2 \in H$ and so $ab = (g_1i)(g_2i) = g_1g_2 \in H$. Hence $H \cup (G\backslash H)i$ is closed and so is a group.

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