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Graphic Representation and Nomenclature of the Four-Dimensional Crystal Classes. IV. Irrational Crypto-Rotation Planes of Non-Crystallographic Orders

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Abstract

The crystallographic symmetry operations in four dimensions that have orders 5, 8, 10 and 12 can be formulated as double rotations of these orders instead of in the ways that have been used previously. The crystallographic character of the operations is compatible with the non-crystallographic orders of their constituent crypto-rotation planes because these lie in crystallographically irrational orientations. The orientations of these planes are derived in terms of the usual crystallographic axes and are illustrated by means of hyperstereograms. The analysis is used to throw further light on the nature, on the enantiomorphy, and on the degrees of freedom of the symmetry operations, but the irrational orientations lead to substantial disadvantages in such a formulation of the symmetry operations for both the graphical and the symbolic representations of the four-dimensional crystal classes.

1. Introduction

Every n-dimensional crystallographic point-group operation can be expressed on a suitable basis in terms of a unimodular square matrix of the form

$$\begin{pmatrix} 1 & 0 & 0 & 0 & 0 & 0 & 0 & 0\ldots \\ 0 & \bar{1} & 0 & 0 & 0 & 0 & 0 & 0\ldots \\ 0 & 0 & \multicolumn{2}{c}{\mathbf{N}_1} & 0 & 0 & 0 & 0\ldots \\ 0 & 0 & & & 0 & 0 & 0 & 0\ldots \\ 0 & 0 & 0 & 0 & \multicolumn{2}{c}{\mathbf{N}_2} & 0 & 0\ldots \\ 0 & 0 & 0 & 0 & & & 0 & 0\ldots \\ 0 & 0 & 0 & 0 & 0 & 0 & \multicolumn{2}{c}{\mathbf{N}_3\ \ldots} \\ 0 & 0 & 0 & 0 & 0 & 0 & & \ldots \end{pmatrix}$$

provided that *either* the first row and column or the second row and column be omitted if n is odd, and both may be omitted if n is even. $\mathbf{N}_i$ is of the form

$$\begin{pmatrix} \cos\theta_i & -\sin\theta_i \\ \sin\theta_i & \cos\theta_i \end{pmatrix}.$$

It may reduce to non-zero diagonal terms (± 1) only if $\theta = 0$ or π. This was already implicit in the work of Hermann (1949), but it has been made explicit by Weigel, Veysseyre, Phan, Effantin & Billiet (1984) that it has the consequence that four-dimensional crystallographic symmetry operations can all be expressed by at most two rotations about absolutely perpendicular planes. Of the fourteen of these operations that leave only a point invariant it has been traditional to describe ten as double rotations, though one of us has introduced an alternative nomenclature (Whittaker, 1984*a*); these ten, with the corresponding alternative notation, are

$$\begin{array}{cccccccccc} \mathbf{22} & \mathbf{32} & \mathbf{42} & \mathbf{62} & \mathbf{33} & \mathbf{66} & \mathbf{44} & \mathbf{63} & \mathbf{43} & \mathbf{64} \\ \tilde{\bar{\mathbf{1}}} & \tilde{\bar{\mathbf{6}}} & \tilde{\bar{\mathbf{4}}} & \tilde{\bar{\mathbf{3}}} & \mathbf{III} & \widetilde{\overline{\mathbf{III}}} & \mathbf{IV} & \mathbf{VI} & \mathbf{XII} & \widetilde{\overline{\mathbf{XII}}}. \end{array}$$

Of the remaining four, two have been traditionally described as multiple rotations: **444** and **3344**, renamed **VIII** and **XII′**. The other two, of order 5 and 10, have not hitherto been regarded as factorizable in this way and were thus the first candidates for the Roman numeral notation **V** and $\tilde{\bar{\mathbf{V}}}$, the latter having also been described in the past as **X**. However, Veysseyre, Phan & Weigel (1985) have now introduced the nomenclature 55, 88, 10,10 and 12,12 for these operations of order 5, 8, 10 and 12 respectively.

Standard forms of the matrices that have been used hitherto (Brown, Bülow, Neubüser, Wondratschek and Zassenhaus, 1978; Whittaker, 1985) for the **V**, $\tilde{\bar{\mathbf{V}}}$, **VIII** and **XII′** operations are given in (1), (3), (4) and (6) below. It is clear from the mathematics that there must exist transformations of axes that convert the more usual forms of the matrices of these operations into the form $\begin{pmatrix} \mathbf{N}_1 & 0 \\ 0 & \mathbf{N}_2 \end{pmatrix}$, where $\mathbf{N}_1$, $\mathbf{N}_2$ are 2×2 matrices for a $2\pi q/p$ rotation in a plane, where p is the order of the operation and q is not a factor of p and may be different for $\mathbf{N}_1$ and $\mathbf{N}_2$. However, this poses a conceptual problem, since a vector lying on either of these planes will be repeated only by the p-fold non-crystallographic rotation symmetry in its

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own plane. We have therefore investigated the orientation of these p-fold planes and their relationship to the graphical representations of the symmetry elements. This is considerably clarified by use of the hyperstereogram (Whittaker, 1973, 1985). Some additional clarification of the degrees of freedom of the symmetry elements (Whittaker, 1985) has also emerged as a result of this work.

2. Equations of the crypto-rotation planes

In general, two successive applications of a symmetry operation to a vector will lead to two images that are not coplanar with the original vector.

However, let $\mathbf{r}$ be a vector and $\mathbf{M}$ a matrix such that $\mathbf{r}$, $\mathbf{M}(\mathbf{r})$ and $\mathbf{M}^2(\mathbf{r})$ all lie in a plane with equal angles θ between $\mathbf{r}$ and $\mathbf{M}(\mathbf{r})$ and between $\mathbf{M}(\mathbf{r})$ and $\mathbf{M}^2(\mathbf{r})$. Let $\mathbf{n}$ be a vector perpendicular to $\mathbf{r}$ in the same plane.

Then since $\mathbf{M}^2(\mathbf{r}) = \lambda\mathbf{r} + \mu\mathbf{M}(\mathbf{r})$ for some λ, μ,

$$\mathbf{M}^2(\mathbf{r}) \,.\, \mathbf{r} = \lambda\mathbf{r} \,.\, \mathbf{r} + \mu\mathbf{M}(\mathbf{r}) \,.\, \mathbf{r}$$

and

$$\mathbf{M}^2(\mathbf{r}) \,.\, \mathbf{n} = \lambda\mathbf{r} \,.\, \mathbf{n} + \mu\mathbf{M}(\mathbf{r}) \,.\, \mathbf{n}.$$

Thus, $\cos 2\theta = \lambda + \mu \cos\theta$ and $\sin 2\theta = \mu \sin\theta$, which give $\mu = 2\cos\theta$, $\lambda = -1$.

Hence,

$$(\mathbf{M}^2 - 2\cos\theta\mathbf{M} + \mathbf{I})\mathbf{r} = \mathbf{0},$$

which defines the plane in which $\mathbf{M}$ has the effect of a rotation through the angle θ.

The appropriate values of θ are given by the equation

$$|\mathbf{M}^2 - 2\cos\theta\mathbf{M} + \mathbf{I}| = 0.$$

The V *operation*

If we take as the standard orientation of the **V** operation that whose matrix referred to the axes of the decagonal or icosagonal systems (Whittaker, 1985, p. 81) is

$$\begin{pmatrix} \bar{1} & 1 & 0 & 0 \\ \bar{1} & 0 & 1 & 0 \\ \bar{1} & 0 & 0 & 1 \\ \bar{1} & 0 & 0 & 0 \end{pmatrix}, \qquad (1)$$

then the above analysis leads to a unique pair of planes whose equations, in terms of these axes, are

$$\Pi_1\colon\quad y = \varphi(x - w), \qquad \varphi z = y - w$$

with $\theta = 72°$ about Π_2, and

$$\Pi_2\colon\quad \varphi y = w - x, \qquad z = \varphi(w - y)$$

with $\theta = 144°$ about Π_1, where $\varphi = (1 + 5^{1/2})/2$. This particular **V** operation is therefore equivalent to that given by a matrix, referred to any orthogonal axes w_0x_0 in Π_1 and any orthogonal axes y_0z_0 in Π_2, of the form

$$\begin{pmatrix} \cos 72° & -\sin 72° & 0 & 0 \\ \sin 72° & \cos 72° & 0 & 0 \\ 0 & 0 & \cos 144° & -\sin 144° \\ 0 & 0 & \sin 144° & \cos 144° \end{pmatrix}. \qquad (2)$$

A four-dimensional crystal possessing this **V** symmetry operation thus has fivefold rotational symmetry on each of these two absolutely perpendicular planes. However, the planes concerned are not rational crystallographic planes. Π_1 is spanned by vectors $[1, \varphi, 1, 0]$ and $[0, 1, \varphi, 1]$, and Π_2 is spanned by vectors $[1, 1, 0, \varphi]$ and $[\varphi, 0, 1, 1]$. There is therefore no translational repetition on these planes, and so there is no reason why the pattern formed by some continuously varying scalar property of the crystal (*e.g.* corresponding to electron density in a three-dimensional crystal) should not have fivefold rotational symmetry on them. This conclusion is, however, somewhat startling to a crystallographer.

It is to be noted, however, that the whole discussion is in terms of point groups, and does not necessarily imply that every section of a structure parallel to Π_1 and Π_2 would have fivefold rotational symmetry. This symmetry would only be expected for sections that contain a point with site symmetry **V**, and such points may not occur in every space group of these crystal classes. We are indebted to one of the referees for pointing this out.

The $\bar{\bar{\mathbf{V}}}$ *operation*

The matrix of a $\bar{\bar{\mathbf{V}}}$ operation in the same orientation as the **V** operation represented by (1) is

$$\begin{pmatrix} 1 & \bar{1} & 0 & 0 \\ 1 & 0 & \bar{1} & 0 \\ 1 & 0 & 0 & \bar{1} \\ 1 & 0 & 0 & 0 \end{pmatrix}. \qquad (3)$$

Since $\bar{\bar{\mathbf{V}}} = \mathbf{V} \,.\, \bar{\bar{\mathbf{1}}}$ and $\bar{\bar{\mathbf{1}}}$ is equivalent to a double twofold rotation on *any* pair of absolutely perpendicular planes, these twofold crypto-rotation planes may be combined with the fivefold crypto-rotation planes to give tenfold crypto-rotation planes in the same orientation. No new principles arise.

The VIII *operation*

If we take the matrix

$$\begin{pmatrix} 0 & 0 & \bar{1} & 0 \\ 0 & 0 & 0 & 1 \\ 0 & 1 & 0 & 0 \\ 1 & 0 & 0 & 0 \end{pmatrix} \qquad (4)$$

as a standard form of the **VIII** operation referred either to the axes of the octagonal system (Whittaker, 1985, p. 81) or to orthogonal axes, then the procedure described above leads to a unique pair of planes containing vectors that are repeated with eightfold symmetry within each plane. Their equations are

$$\Pi_1: \quad w-x+y2^{1/2}=0, \qquad w+x-z2^{1/2}=0$$

with $\theta=45°$ about Π_2, and

$$\Pi_2: \quad w-x-y2^{1/2}=0, \qquad w+x+z2^{1/2}=0$$

with $\theta=135°$ about Π_1. Π_1 is spanned by $[0,2^{1/2},1,1]$ and $[2^{1/2},0,\bar{1},1]$, and Π_2 by $[0,2^{1/2},\bar{1},1]$ and $[2^{1/2},0,1,\bar{1}]$, so that again they are irrational planes. They are therefore not constrained by translational repetition, and may exhibit eightfold rotational symmetry analogous to the fivefold symmetry discussed above. The matrix with respect to any orthogonal axes w_0x_0 lying in Π_1 and y_0z_0 in Π_2 is

$$\begin{pmatrix} 1/2^{1/2} & -1/2^{1/2} & 0 & 0 \\ 1/2^{1/2} & 1/2^{1/2} & 0 & 0 \\ 0 & 0 & -1/2^{1/2} & -1/2^{1/2} \\ 0 & 0 & 1/2^{1/2} & -1/2^{1/2} \end{pmatrix}. \tag{5}$$

A notation for the irrational orientations of the eightfold crypto-rotation planes in the hypercubic system has been given previously by Veysseyre, Weigel, Phan & Effantin (1984).

The XII′ *operation*

The particular orientation of the **XII′** operation represented by

$$\begin{pmatrix} 0 & \bar{1} & 0 & 1 \\ 1 & 0 & \bar{1} & 0 \\ 0 & \bar{1} & 0 & 0 \\ 1 & 0 & 0 & 0 \end{pmatrix} \tag{6}$$

with respect to the axes of the dodecagonal system (Whittaker, 1985, p. 81*) can be shown in the same way to be equivalent to a unique pair of crypto-rotation planes with equations

$$\Pi_1: \quad w-2y=x3^{1/2}, \qquad 2z-x=w3^{1/2}$$

with $\theta=30°$ about Π_2, and

$$\Pi_2: \quad 2y-w=x3^{1/2}, \qquad x-2z=w3^{1/2}$$

with $\theta=150°$ about Π_1. Again, these planes are spanned by irrational vectors, $[2,0,1,3^{1/2}]$ and $[0,2,-3^{1/2},1]$ for Π_1 and $[2,0,1,-3^{1/2}]$ and $[0,2,3^{1/2},1]$ for Π_2, so that similar conclusions hold good.

* In the reference given, the angle xy, given as γ, should be $180°-\gamma$.

3. Graphical representation of the V and $\tilde{\tilde{\mathbf{V}}}$ operations

One of us has discussed previously (Whittaker, 1984*a*, 1985) an extension of the concept of 'symmetry element' that is convenient in the present work. In the strict sense a symmetry element is the locus of points that are invariant under the action of a symmetry operation, and for any double rotation in four dimensions this is merely a point. In an extended sense, however, we describe as the symmetry element the whole complex of ideas that associates this point, the order of the operation, the geometrical specification of directional parameters associated with it, and its representation by a suitable graphical symbol in a hyperstereogram. Such representations for double rotations have been by means of their constituent crypto-rotation planes if these were uniquely defined, and the above discussion shows that this would now be possible for the **V**, $\tilde{\tilde{\mathbf{V}}}$, **VIII** and **XII′** operations. Up to now their symmetry elements have been represented by a small-scale hyperstereographic diagram below the main hyperstereogram showing the effect of the operation on the crystallographic axes. Both representations are used in Figs. 1–10, which illustrate the relations between them and the rather complementary information that they convey.

In Fig. 1 the positions of Π_1 and Π_2 are shown for the **V** operations corresponding to matrix (1) above related to the axes of the icosagonal system (system 31). In Fig. 1(a) a point labelled A has been taken close to the chain line representing the plane Π_1; application of the operation to point A leads to point B, and this involves a rotation of $4\pi/5$ about the line combined with a movement of $2\pi/5$ along it, *i.e.* about the plane Π_2 represented by the other chain line. Repeated application takes B to C and then to the negative points D and E in the expected way. In Fig. 1(b) the point A has been taken close to the chain line representing Π_2, and one application of the operation therefore takes it to B by a rotation of $2\pi/5$ about it and $4\pi/5$ along it, and further applications lead to C, D and E. However, the distinction would be much less obvious if the points were not labelled. The successive points along the Π_2 chain line, *ADBEC* in Fig. 1(b), differ only from those along the Π_1 chain line *ABCDE* in Fig. 1(a) by the sense of their rotation about the chain line to which they are close; in (a) they follow a left-handed helix and in (b) a right-handed helix.

In Fig. 1(c) the points have been taken on Π_1 so that they represent five coplanar vectors with the anomalous pentagonal symmetry on a crystallographically irrational plane.

In the hyperstereograms of Fig. 1 it is to be noted that the chain line representing the positive half of each crypto-rotation plane intersects (in three dimensions) the broken line representing the negative

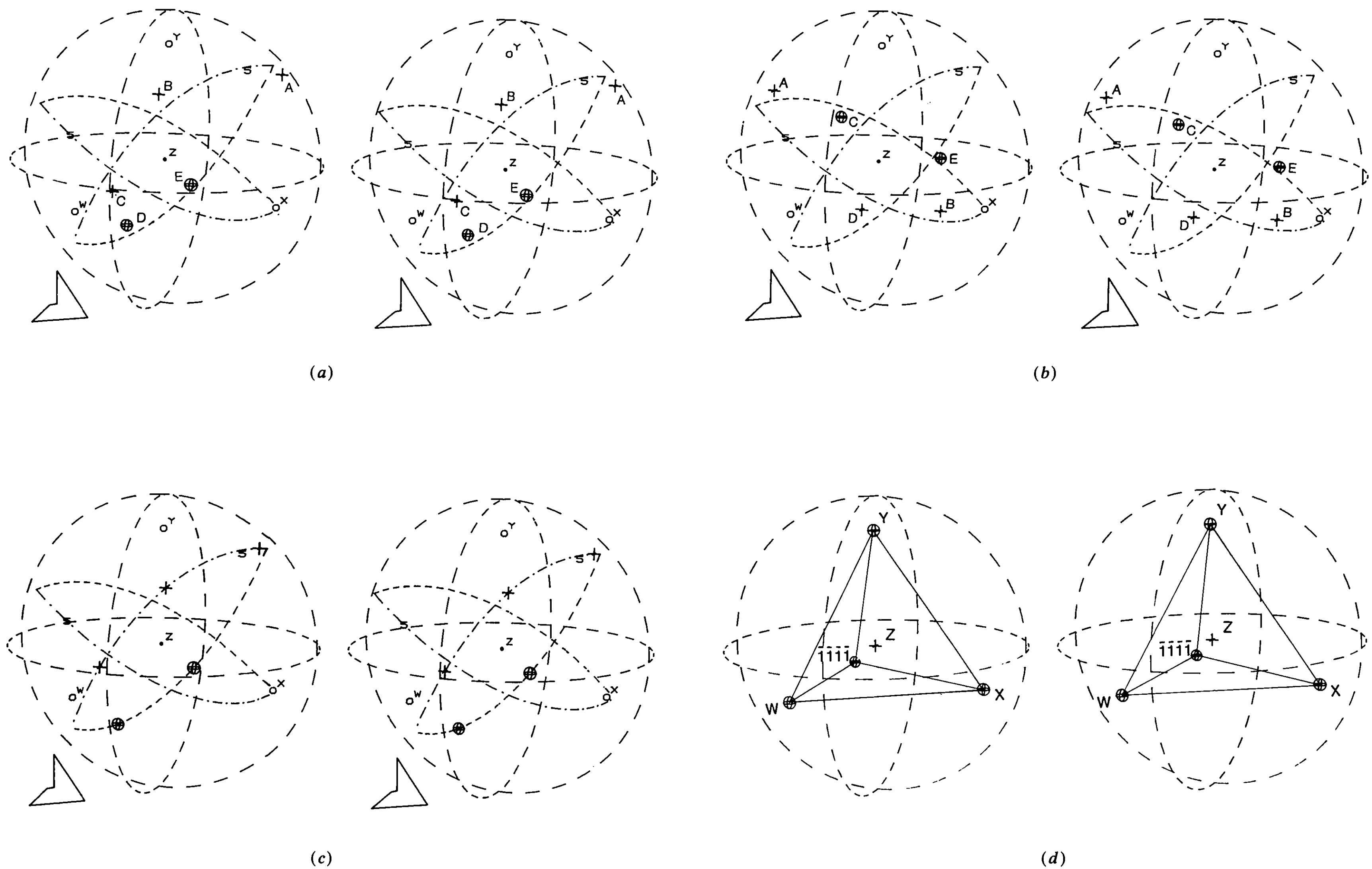


Fig. 1. The pentatope operation that converts $z \to y \to x \to w \to [\bar{1}\bar{1}\bar{1}\bar{1}]$ shown in terms of its crystallographically irrational crypto-rotation planes of order 5 referred to the axes of the icosagonal system. (*a*) Successive applications of the operation to point A convert it to B, C, D, E related by 144° left-handed screw rotations along the adjacent chain line which represents Π_1. (*b*) Successive applications of the operation to point A adjacent to Π_2 leads by 72° screw rotations to B, C, D, E; but the sequence of points $ADBEC$ again corresponds to 144° screw rotations about the adjacent chain line, although the screw is right handed. (*c*) Five coplanar vectors on Π_1 related by a fivefold rotation, and represented by points on the chain line. (*d*) The tetrahedron formed by joining all six pairs of the points representing w, x, y and $[\bar{1}\bar{1}\bar{1}\bar{1}]$.

half of the absolutely perpendicular plane projected to the north pole. The existence of this intersection arises from the fact that each of the planes Π_1 and Π_2 makes an angle of 45° with the z axis. The straight line joining these two intersections passes through z and represents the plane containing [1100] and $[\bar{1}\bar{1}0\bar{1}]$. In the hyperstereogram it is the join of the mid-points of two opposite edges of the tetrahedron with vertices at w, x, y and $[\bar{1}\bar{1}\bar{1}\bar{1}]$ shown in Fig. 1(d), and this join is one of the (three-dimensional) $\bar{4}$ axes of this tetrahedron. The tetrahedral symbol of the **V** operation shown at the lower left of the hyperstereograms is based on a copy of this tetrahedron on a smaller scale (and including the point representing the z axis at its centre) in which the joins indicate the effects in sequence that the operation has on the axes; in the symbol the join of [1100] and $[\bar{1}\bar{1}0\bar{1}]$ is uniquely defined as joining the mid-point between two vertices that are both joined to z and the mid-point between two vertices that are neither joined to z. This definition is independent of the convention as to which power of the operation is directly represented by the symbol, and it is invariant for all its powers.

The four-dimensional equivalent of the above statement is that the hyperplanes $z\Pi_1$ and $z\Pi_2$ intersect in the plane $z[1100]$.

Fig. 1 is constructed with the axes w, x, y, z of the icosagonal system (Whittaker, 1985, p. 81) in which all the inter-axial angles are equal to $\cos^{-1}(-\frac{1}{4})$. In the more general case of the decagonal system the six interaxial angles fall into two groups of three; if the pentatope operation converts $z\to y\to x\to w\to [\bar{1}\bar{1}\bar{1}\bar{1}]$ then these are

$$w\hat{\ }x \equiv x\hat{\ }y \equiv y\hat{\ }z = \theta$$

and

$$w\hat{\ }y \equiv x\hat{\ }z \equiv z\hat{\ }w = \varphi$$

such that

$$\cos\theta + \cos\varphi = -0{\cdot}5.$$

Fig. 2(a) has been constructed for $\theta = 90°$, $\varphi = 120°$, and it may be seen that the representation of Π_1 is then less than 45° from z, while that of Π_2 is correspondingly more than 45° from z; and they do not intersect. In Fig. 2(b) $\theta = 74{\cdot}57°$, $\varphi = 140°$, and the representation of Π_1 is quite close to the polar axis of the hyperstereogram while that of Π_2 is quite close to the equator.

The limit of this change of θ and φ would be when $\theta = 72°$, $\varphi = 144°$. In this limit Π_1 would coincide with the yz plane and would also contain the w and x axes. Thus the four-dimensional space would have degenerated into two dimensions. The opposite limit would of course be with $\theta = 144°$, $\varphi = 72°$; in this case Π_2 would contain all four axes. The case with $\theta = \varphi = \cos^{-1}(-\frac{1}{4})$ is half way between the two limits.

It is to be noted that the intersection of the hyperplanes $z\Pi_1$ and $z\Pi_2$ in the plane $z[1100]$ is independent of the values of θ and φ. In the limit where the four dimensions degenerate to two this plane degenerates to the z axis.

Fig. 3 shows a hyperstereogram of a $\bar{\bar{\mathbf{V}}}$ operation and its crypto-rotation planes of order 10. It is identical with Fig. 1(a) except for the addition of a $\bar{\bar{1}}$ operation which leads to the duplication of each point (w, x, y, z) by its opposite ($\bar{w}$, $\bar{x}$, $\bar{y}$, $\bar{z}$). No new features arise.

4. Graphical representation of the VIII operation

The phenomena that arise in this case are very similar to those in § 3, with one exception. The operation is again possible in two crystal systems: the octagonal here is oriented* so that

$$w\hat{\ }x = y\hat{\ }z = 90°$$

and

$$x\hat{\ }y = x\hat{\ }z = z\hat{\ }w = 180° - w\hat{\ }y;$$

and the hypercubic is oriented with all axes orthogonal. Again, the axes of the higher-symmetry system correspond to a position half way through the permissible range of variation in the lower-symmetry system. This ranges from a lower limit of $w\hat{\ }y = 45°$ to an upper limit of $w\hat{\ }y = 135°$, and at both limits the four-dimensional arrangement degenerates to a two-dimensional one.

Figs. 4(a), (b) and (c) show the situation when the axes are orthogonal and the points are close to Π_1, close to Π_2 and on Π_1, respectively. Successive applications of the operation lead to the sequence of points *ABCDEFGH* which follow a left-handed helix round Π_1 in (a), with a 135° turn per application. In (b) successive applications give *ABCDEFGH* with a 45° turn along a left-handed helix of three times the pitch, but consecutive points *ADGBEHCF* follow a helix round Π_2 identical to that followed by consecutive points round Π_1 in (a). Thus the overall effect of both crypto-rotation planes is identical.

Figs. 5(a) and (b) show the effect of changing the interaxial angles; in (a) the non-orthogonal angles are 70° (three angles) and 110° ($w\hat{\ }y$), and in (b) they are 50° (three angles) and 130° ($w\hat{\ }y$). The latter clearly shows the approach to the limit when all the axes would be coplanar and lie on Π_1, the polar axis of the hyperstereogram.

As in the case of the **V** operation, the hyperplanes $z\Pi_1$ and $z\Pi_2$ intersect in the plane $z[1100]$, and at the middle of the permitted range of interaxial angles (which here corresponds to all axes orthogonal) the planes Π_1 and Π_2 are both at 45° to z.

* This orientation is obtained from that illustrated on p. 148 of Whittaker (1985) by converting x to y and y to x.

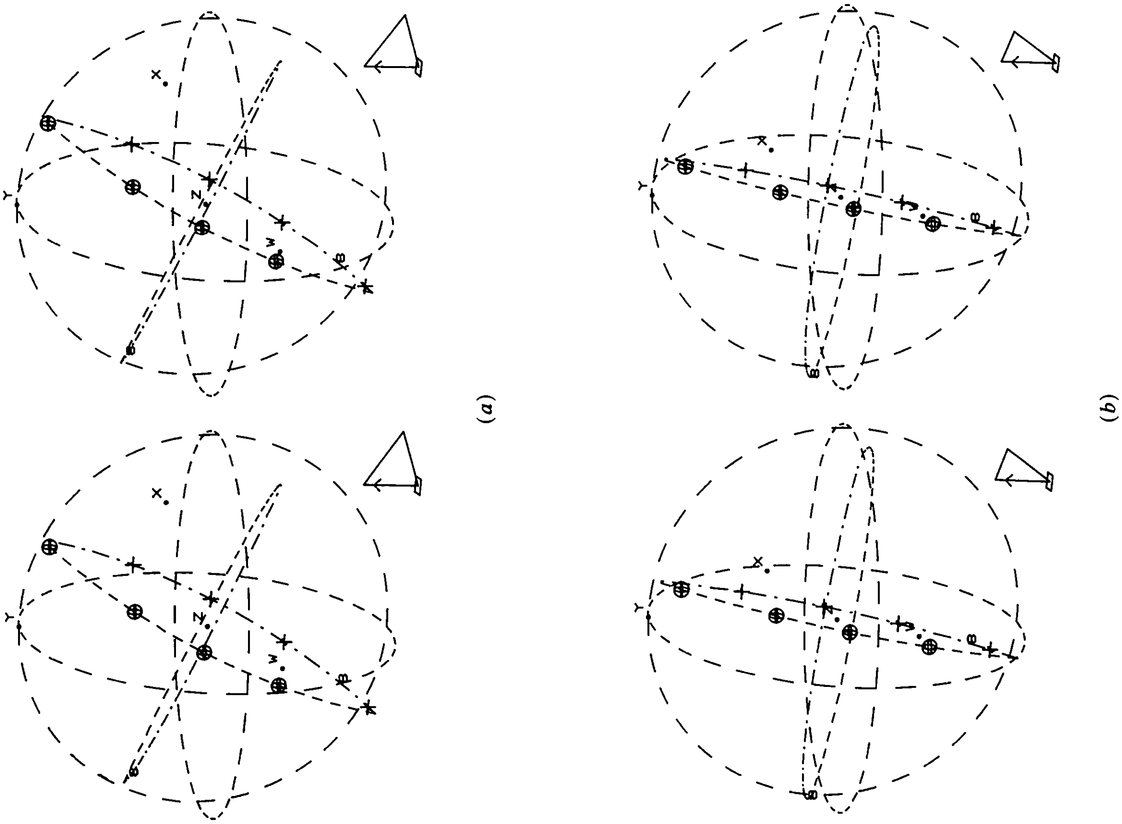


Fig. 5. The same operation as in Fig. 4 (on p. 393) referred to the axes of the octagonal system. (a) $x\hat{}y = x\hat{}z = z\hat{}w = 70°$; $w\hat{}y = 110°$. (b) $x\hat{}y = x\hat{}z = z\hat{}w = 50°$; $w\hat{}y = 130°$.

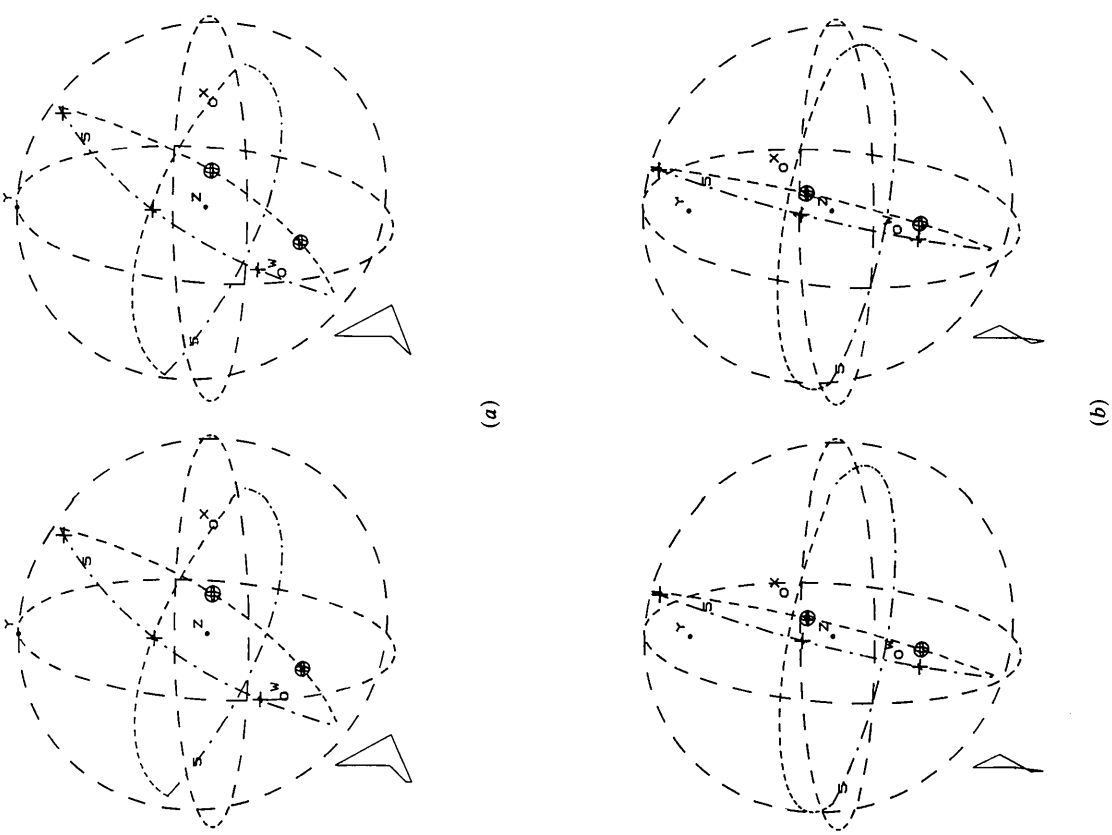


Fig. 2. The same operation as in **Fig.** 1 referred to the axes of the decagonal system, with $\theta = w\hat{}x = x\hat{}y = y\hat{}z$; $\varphi = w\hat{}y = x\hat{}z = z\hat{}w$. (a) $\theta = 90°$, $\varphi = 120°$. (b) $\theta = 74{\cdot}57°$, $\varphi = 140°$.

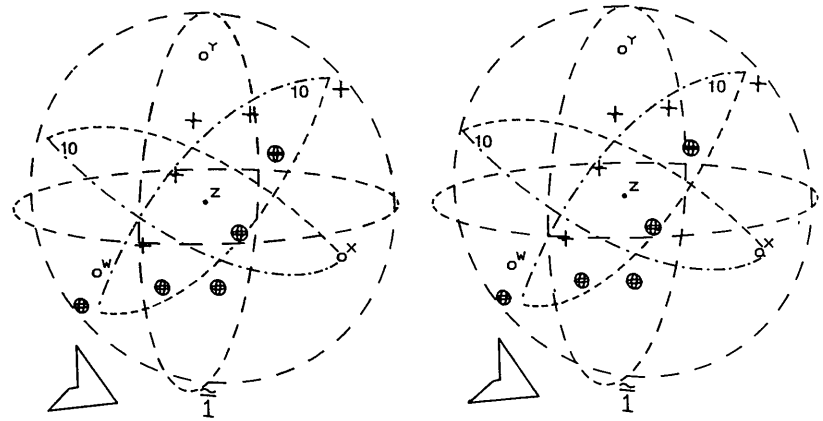
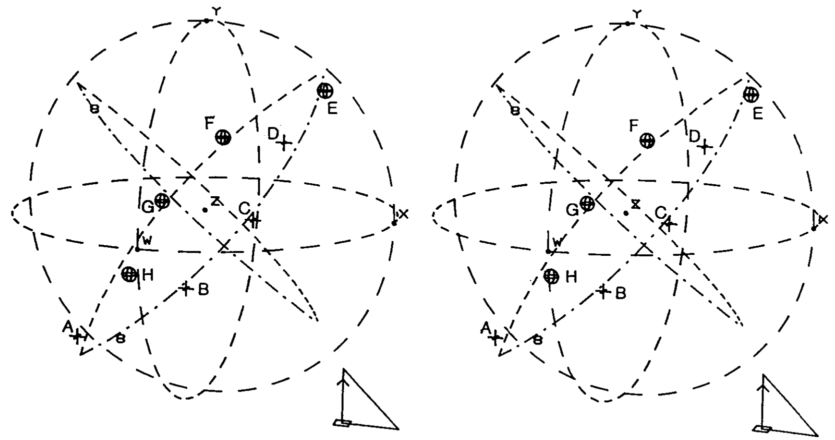
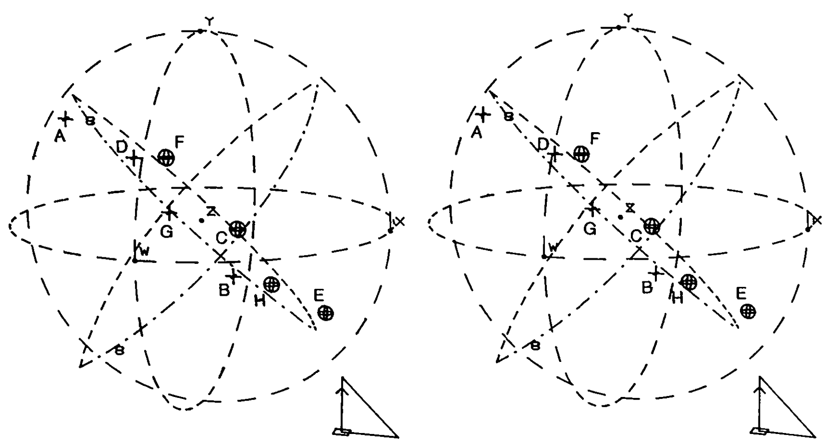


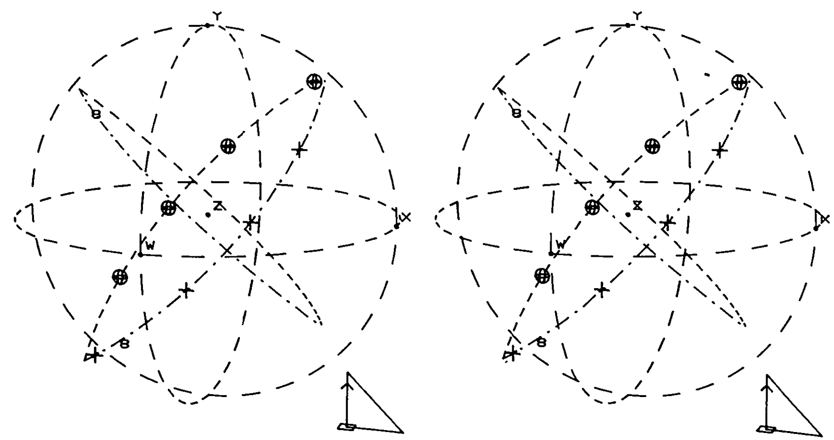
Fig. 3. The $\tilde{\mathbf{V}}$ operation analogous to Fig. 1(a), with the crystallographically irrational crypto-rotation planes of order 10 referred to the axes of the icosagonal system.



(a)



(b)



(c)

Fig. 4. The **VIII** operation that converts $z \to x \to y \to w \to \bar{z} \to \bar{x} \to \bar{y} \to \bar{w}$, shown in terms of its crystallographically irrational crypto-rotation planes of order 8, referred to orthogonal axes. (a) Points in alphabetical order near the representation of Π_1 represent successive applications of the operation and follow a left-handed helix with a 135° turn between each one. (b) Points near the representation of Π_2 follow a different helix if taken in order of successive applications of the symmetry operation (alphabetical order) but constitute an array whose successive points follow a similar helix to (a). (c) Points on Π_1, representing a set of eight coplanar vectors related by an eightfold rotation.

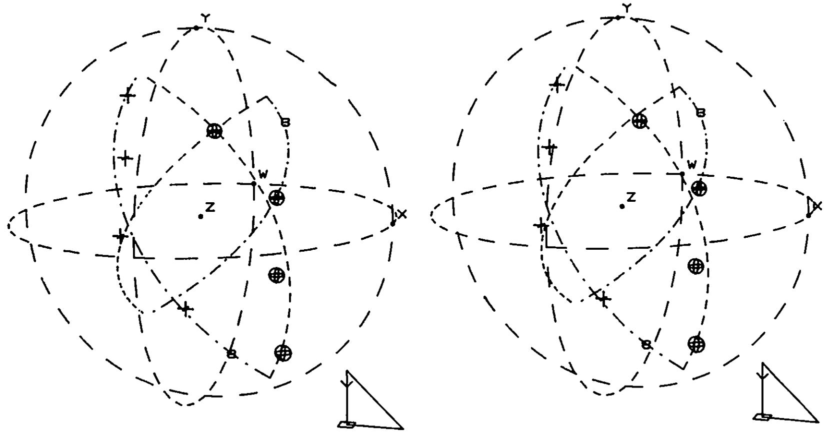
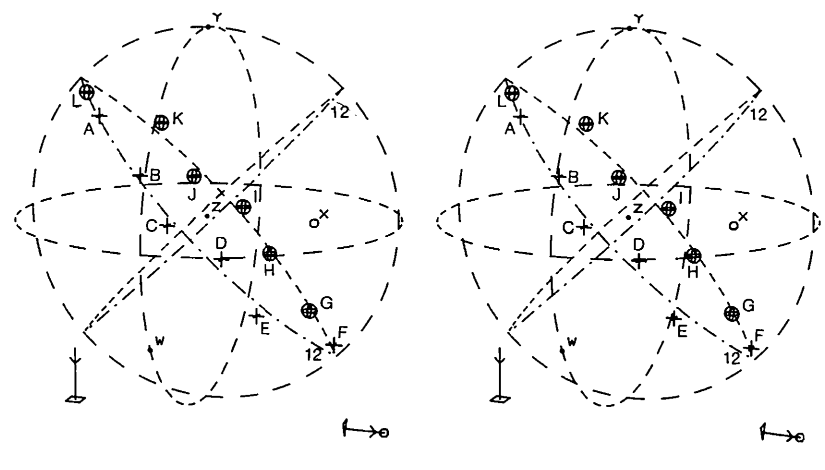
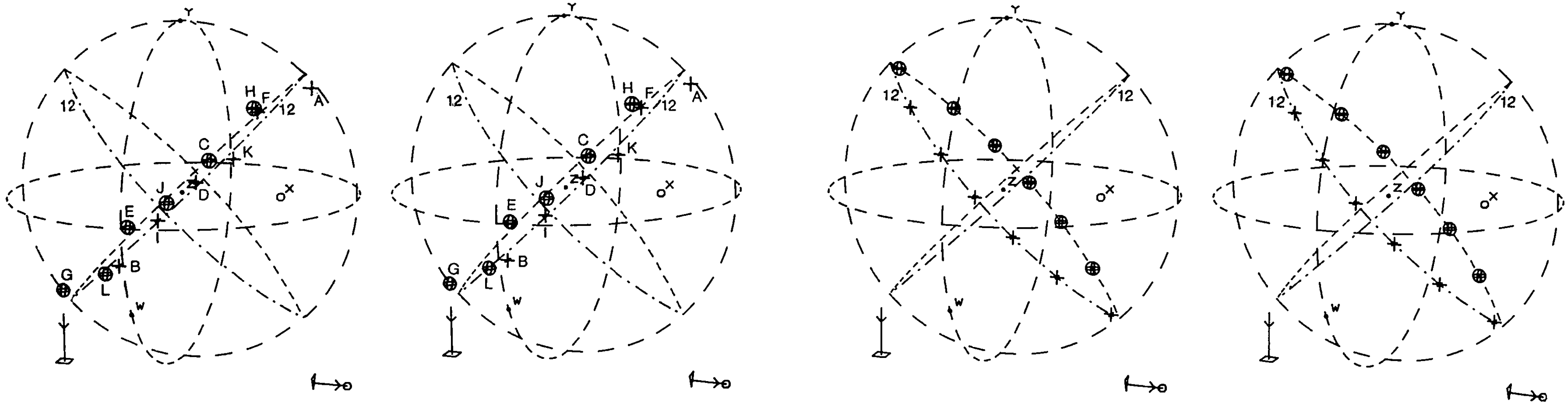


Fig. 6. The enantiomorphic form of the operation shown in Fig. 4(b). The points follow a right-handed helix.



(a)



(b) (c)

Fig. 7. The **XII'** operation that converts $z \to w \to [0101] \to y \to x \to [\bar{1}0\bar{1}0] \to z \to w \to [0\bar{1}0\bar{1}] \to y \to x \to [1010]$, shown in terms of its crystallographic irrational crypto-rotation planes of order 12, referred to axes of the dodecagonal system in the special case where $w\hat{}z = x\hat{}y = 90°$. ($a$) Points in alphabetical order near the representation of Π_1 represent successive applications of the operation and follow a left-handed helix with a 150° turn between each one. (b) Points near the representation of Π_2 follow a different helix if taken in order of successive applications of the symmetry operation (alphabetical order) but constitute an array whose successive points follow a similar helix to (a). (c) Points on Π_1 representing a set of twelve coplanar vectors related by a 12-fold rotation.

The fact that the points in the hyperstereograms follow helices of the same hand round Π_1 and Π_2 corresponds to the fact that the **VIII** operation is enantiomorphic, whereas the **V** operation is not enantiomorphic and helices of both hands are present in its hyperstereogram. Fig. 6 corresponds to Fig. 4(*b*) but in the enantiomorphic form.

5. Graphical representation of the XII′ operation

This operation is described in terms of the axes of the dodecagonal system which require

$$w^\wedge x = y^\wedge z = 90°, \qquad w^\wedge y = x^\wedge z = 120°$$

and two angles left undefined, but related by*

$$w^\wedge z = 180° - x^\wedge y.$$

The permitted range of these two angles is from 30 to 150° and at both limits the four axes become coplanar. No higher symmetry is attained at the centre of the range where $w^\wedge z = x^\wedge y = 90°$, but the component **IV** and **III** operations then have their symbols at right angles. This situation is shown in Fig. 7. Points close to the planes Π_1 and Π_2 form similar arrays on screws of the same hand in the same way as in Fig. 4, although again different sequences of points are produced by successive applications of the symmetry operation. The effect of changing $x^\wedge y$ from 90 to 65 and to 40° is shown in Fig. 8. In the limiting condition the symbols of the component **IV** and **III** operations would be parallel to one another. The enantiomorph of Fig. 7(*a*) is shown in Fig. 9, and the points follow a right-handed helix.

The hyperplanes $z\Pi_1$ and $z\Pi_2$ intersect in the plane $z[2010]$, which is represented in the hyperstereogram by the diameter of the equator perpendicular to the plane containing the x, y and z points.

6. Interchange of crypto-rotation planes

In the formulation of a **V** operation as a **55** double rotation the trace of the matrix must be -1. This is satisfied if the rotation angle in the upper-left quadrant of the matrix is 72° and that in the lower-right quadrant is 144°, since

$$\cos 72° = (5^{1/2} - 1)/4 \text{ and } \cos 144° = (-5^{1/2} - 1)/4,$$

so that

$$\operatorname{trace}(M) = 2\cos 72° + 2\cos 144° = -1.$$

*This relationship is incorrectly given as $w^\wedge z = x^\wedge y$ on pp. 81 and 151 of Whittaker (1985).

It would also be satisfied if the angle at lower right were 216°, but since

$$\begin{pmatrix} \cos 72° & -\sin 72° & 0 & 0 \\ \sin 72° & \cos 72° & 0 & 0 \\ 0 & 0 & \cos 216° & -\sin 216° \\ 0 & 0 & \sin 216° & \cos 216° \end{pmatrix}^2 = \begin{pmatrix} \cos 144° & -\sin 144° & 0 & 0 \\ \sin 144° & \cos 144° & 0 & 0 \\ 0 & 0 & \cos 72° & -\sin 72° \\ 0 & 0 & \sin 72° & \cos 72° \end{pmatrix}$$

this is equivalent to interchanging the angles on the two planes.

The process of derivation of the planes Π_1 and Π_2 from the operation **V** in § 2 unequivocally assigned the 72° angle to one plane and the 144° to the other. However, there must exist another **V** operation ($\mathbf{V}_{\text{int}}$) that has the same pair of crypto-rotation planes but with the rotation angles interchanged. Fig. 10 shows the effect of this $\mathbf{V}_{\text{int}}$ operation with the points near Π_1 in its alternative position, *i.e.* the position of Π_2 in Fig. 1(*a*). The graphical symbol of the $\mathbf{V}_{\text{int}}$ operation shows the totally different orientation of the effect that the operation has on the z axis.

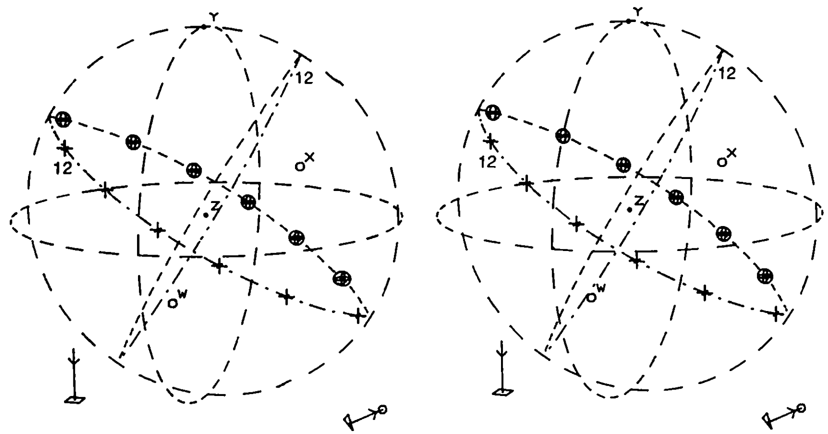
The product of **V** and $\mathbf{V}_{\text{int}}$ is an explicit fivefold rotation plane. These two operations cannot coexist in any crystal class, as is evident from the fact that the orientation of $\mathbf{V}_{\text{int}}$ is irrational with respect to the crystallographic axes appropriate to **V**.

In the formulation of $\tilde{\mathbf{V}}$ as a **10,10** double rotation the same problem arises. The two angles are 36 and 108° and must be a specific way round for a particular $\tilde{\mathbf{V}}$ operation. Since $\tilde{\mathbf{V}}$ contains an explicit **V** among its powers exactly the same considerations arise.

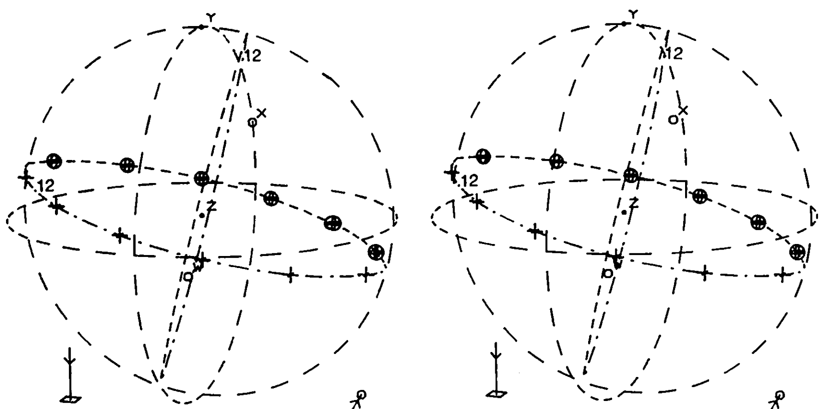
In the formulation of **VIII** and **XII′** as double rotations the problem does not arise, because in both of them interchange of rotation angle merely leads to a power of the same operation.

7. Degrees of freedom of the operations

It has previously been deduced from the characteristics of the geometrical symbols required to specify the **V**, $\tilde{\mathbf{V}}$, **VIII** and **XII′** operations that they have four degrees of orientational freedom (Whittaker, 1985). This is confirmed by the present analysis, since a plane (Π_1) has these degrees of freedom. However, in terms of both analyses, one of these degrees of freedom seems at first sight to be different from the others in that it depends on the value of a variable interaxial angle or set of interaxial angles. This apparently peculiar feature arises because we have adopted the convention of always placing the z point at the centre of the hyperstereogram. The matter may be clarified by comparing the situation depicted in



(a)



(b)

Fig. 8. The same operation as in Fig. 7 but referred to general axes of the dodecagonal system. (a) $x\hat{\ }y=65°$, $w\hat{\ }z=115°$. (b) $x\hat{\ }y=40°$, $w\hat{\ }z=140°$.

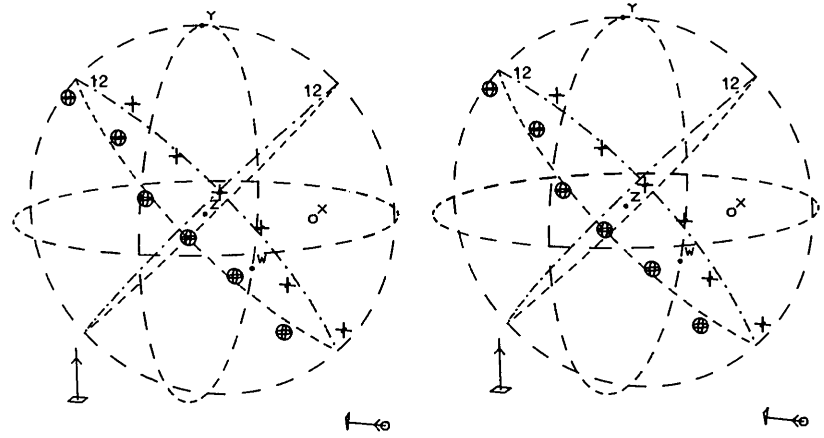


Fig. 9. The enantiomorphic form of the operation shown in Fig. 7(b). The points follow a right-handed helix.

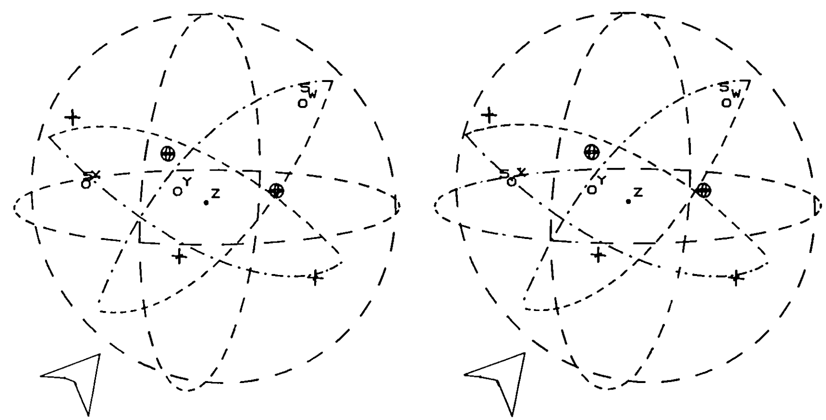


Fig. 10. The equivalent of Fig. 1(a) with the orientations of Π_1 and Π_2 interchanged. The orientation of the graphical symbol for V shows the changed effect of the operation on the z axis.

Figs. 1 and 2 with comparable situations in lower dimensions.

The **V** operation in four dimensions belongs to a series in spaces of increasing dimensionality, as shown by the following sequence of matrices

$$\begin{pmatrix}\bar{1} & 1\\ \bar{1} & 0\end{pmatrix},\quad \begin{pmatrix}\bar{1} & 1 & 0\\ \bar{1} & 0 & 1\\ \bar{1} & 0 & 0\end{pmatrix},\quad \begin{pmatrix}\bar{1} & 1 & 0 & 0\\ \bar{1} & 0 & 1 & 0\\ \bar{1} & 0 & 0 & 1\\ \bar{1} & 0 & 0 & 0\end{pmatrix},$$

$$\begin{pmatrix}\bar{1} & 1 & 0 & 0 & 0\\ \bar{1} & 0 & 1 & 0 & 0\\ \bar{1} & 0 & 0 & 1 & 0\\ \bar{1} & 0 & 0 & 0 & 1\\ \bar{1} & 0 & 0 & 0 & 0\end{pmatrix}, \quad \ldots.$$

In two dimensions we have a threefold rotation, in three dimensions a $\bar{4}$ rotation inversion, and in four dimensions a **V** operation which is a **55** double rotation. In general, in n dimensions we have

$n=2m$: m crypto-rotations on absolutely perpendicular planes through angles $2\pi k/(n+1)$, with $k=1,\ldots,m$;

$n=2m+1$: m crypto-rotations as above combined with a crypto-mirror perpendicular to a direction orthogonal to all of them.

When the number of dimensions is four or less we can bring out the relationships by geometric illustrations. The next two members of the sequence (in five and six dimensions) will have crypto-operations which may be indicated by the symbols **63m** and **777** (by analogy with **55**).

The two-dimensional threefold-rotation point clearly has no degrees of freedom of orientation. Its appropriate crystallographic axes are z and y at 120° to one another and a third axis $[\bar{1}\bar{1}]$ making 120° with both. The **3** operation repeats $z\rightarrow y\rightarrow[\bar{1}\bar{1}]\rightarrow z$, and it also repeats any arbitrary vector to generate the vertices of an equilateral triangle. Although there is no difficulty in drawing a diagram showing all these features on a plane it is instructive to draw a 'hypostereogram'. This is a projection of points on the unit circle on to a diameter by joining them to the 'south pole of the circle', with the result shown in Fig. 11. If the z axis is conventionally projected to the centre of the hypostereogram then the y axis and $[\bar{1}\bar{1}]$ necessarily appear in the positions shown because of the lack of any degree of freedom.

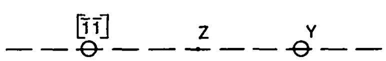


Fig. 11. A hypostereogram of the crystallographic 120° axes appropriate to the two-dimensional **3** rotation operation.

The **4** operation represented by

$$\begin{pmatrix}\bar{1} & 1 & 0\\ \bar{1} & 0 & 1\\ \bar{1} & 0 & 0\end{pmatrix}$$

is in terms of axes from the centre to the vertices of a tetrahedron (not necessarily regular), these directions being the z, y, x and $[\bar{1}\bar{1}\bar{1}]$ axes. It successively transforms $z\rightarrow y\rightarrow x\rightarrow[\bar{1}\bar{1}\bar{1}]\rightarrow z$. In the ordinary stereogram (Fig. 12) we again use the convention that z is at the centre. If the tetrahedron is regular the other axes appear on a circle round z at a radius of 109° 28′, and we can draw a subsidiary stereographic figure to represent the sequence of operations. We can also put in the position of the $\bar{4}$ axis which must be on the bisector of zx, *i.e.* on a circle of radius 54° 44′ around z. Thus the $\bar{4}$ operation is restricted to one degree of freedom (its position round this circle) if we maintain z in the centre and require the axes to remain those of a regular tetrahedron, whereas the $\bar{4}$ axis is known to have two degrees of orientational freedom. The second one is regained if it is allowed to change its distance from z, and so to give rise to the axes of a tetrahedron that is not regular, but has two interaxial angles θ and four interaxial angles φ with the restriction

$$\cos\varphi+\tfrac{1}{2}\cos\theta=-\tfrac{1}{2}.$$

The result (with $\theta=80°$) is shown in Fig. 13. Obviously this $\bar{4}$ operation still generates a regular tetrahedron if a representative point is put at the appropriate angle of 54° 44′ from the fourfold crypto-axis. The graphical symbol in terms of the crystal axes has changed but the operation is unchanged except in orientation.

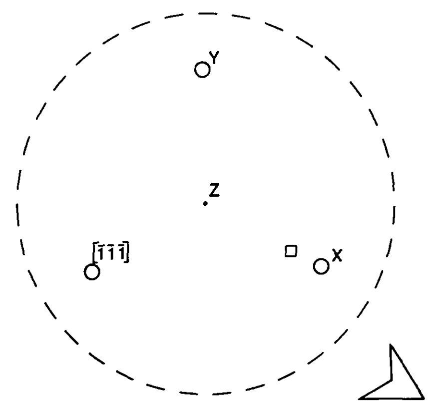


Fig. 12. A stereogram of the axes from the centre to the vertices of a regular tetrahedron. The position of the crypto-rotation axis of one of the $\bar{4}$ operations is shown. The subsidiary stereographic diagram shows the effect of successive operations of this on the z point of the stereogram.

The situation is thus directly analogous to that regarding the degrees of freedom of the **V** operation in four dimensions. With the z point defined to be at the centre of the hyperstereogram the fourth degree of freedom is only obtained by distorting the axes from regularity and correspondingly distorting the graphical symbol, but again this does not prevent the operation from generating a regular pentatope from an appropriately oriented vector that makes 45° with both the crypto-rotation planes. The symmetry operation is the same but its component crypto-rotation planes are differently oriented with respect to the crystal.

The situation in the $\tilde{\tilde{\mathbf{V}}}$, **VIII** and **XII′** operations does not seem to be susceptible of so direct a comparison with symmetry in spaces of lower dimensionality, but it is obviously open to the same explanation.

8. Concluding remarks

Since it is known that the **V**, $\tilde{\tilde{\mathbf{V}}}$, **VIII** and **XII′** operations can all be formulated as double rotations of the appropriate orders, 5, 10, 8 and 12 respectively, it follows that any structure subject to one of these symmetry operations possesses exact rotational symmetry of such an order on certain planes. However, this is shown to be compatible with the existence of a four-dimensional lattice because the planes in question are crystallographically irrational and so do not themselves exhibit any translational repetition.

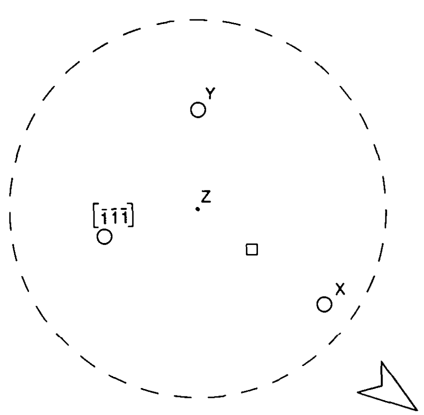


Fig. 13. A corresponding stereogram to Fig. 12 if the axes point to the vertices of an irregular tetrahedron having $\bar{4}$ symmetry along the bisector of the angle between the z and x axes. The crypto-rotation axis makes a different angle with z (here 40° instead of 54° 44′), and the subsidiary diagram is correspondingly distorted.

Formulation of these symmetry operations as double rotations, and representation of their crypto-rotation planes in hyperstereograms, greatly clarifies their geometrical nature and some features of their degrees of orientational freedom and enantiomorphism. However, both because of the irrational orientations of the crypto-rotation planes and of the complicated character of the operations it is very difficult to deduce, from the representation of the crypto-rotation planes, the effects of the operation on the crystallographic axes. It is necessary to be able to deduce these effects in order to relate the hyperstereographic representation of the point group to its generating matrices, and the previously introduced subsidiary graphical symbols therefore continue to be preferred for many purposes. Furthermore, the irrational orientations also mean that the double rotation notation (*e.g.* **55**) is not readily compatible with the Hermann–Mauguin-type notation for the crystal classes proposed by Whittaker (1984*b*, 1985) in which symbol positions are associated with crystallographic planes and directions.

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