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Graphic Representation and Nomenclature of the Four-Dimensional Crystal Classes. II. The Individual Symmetry Operations

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Abstract

The nature of the four-dimensional crystallographic symmetry operations is clarified by representation of their effects in hyperstereograms presented in the form of stereo-pairs. Appropriate graphical symbols have been devised to indicate the orientations of the corresponding symmetry elements. Typographical symbols have been devised for the operations themselves, and for their symmetry elements, which are adaptable for use in a system of symbolic nomenclature of the four-dimensional classes following the general principles of the Hermann–Mauguin notation.

Introduction

Paper I of this series (Whittaker, 1983) reviewed the general nature of the four-dimensional symmetry operations, and the classification of their symmetry elements into mirror hyperplanes, rotation planes, rotation–inversion axes, and point symmetry elements. It also presented hyperstereograms and Hermann–Mauguin-style symbols for the sixteen crystal classes (belonging to the first six crystal systems) that contain symmetry operations of order not greater than two. Preparation of hyperstereograms of all the 227 geometric crystal classes of four dimensions has now been completed, and these will be published elsewhere (Whittaker, 1984). It is the purpose of the present paper to elucidate further, by means of hyperstereograms, the nature of the symmetry operations of order greater than two, and to show how their symmetry elements may be represented symbolically. The representation of a mirror hyperplane in a general orientation (which did not occur in the 16 classes in paper I) is also illustrated.

It is helpful to distinguish a symmetry operation (which can be equated to its matrix representation) from the corresponding symmetry element by the use of bold type. Thus **m** is a reflection operation and *m* is (in four dimensions) a mirror hyperplane.

In the hyperstereograms in this paper the positions of orthogonal axes have been indicated (except in Fig. 16). These are not intended as the crystallographic axes of any particular crystal systems, and are included solely for ease of reference. In Fig. 16 the discussion is simplified by the use of non-orthogonal axes, which are in fact those appropriate to system 27 (the decagonal) of Brown, Bülow, Neubüser, Wondratscheck & Zassenhaus (1978).

Mirror hyperplanes

It has been shown previously (Whittaker, 1973*a*) that mirror hyperplanes are represented in the hyperstereogram by the primitive itself, by a diametral plane, or by a spherical cap that intersects the primitive in a great circle. The first two kinds of representation occur, and their mode of operation has been discussed, in paper I: on the primitive in class No. 3 (2/01, class *m*), and on all three axial planes in No. 14 (6/01, class *mmm*). To represent a spherical cap two dotted circles lying on the cap are used as in Fig. 1, in which the cap intersects the primitive on the equator *wx*. To construct the reflection of a given point in such a cap one considers a central plane of the hyperstereogram through the point and perpendicular to the great circle in which the cap intersects the primitive. One can then treat this section as an ordinary stereogram. Its intersection with the cap behaves exactly as if it were the representation of a mirror plane in such a stereogram.

Rotation planes

Rotation planes, like mirror hyperplanes, are represented in the hyperstereogram in three forms, by a great circle of the primitive, by a diameter of the primitive, and by a circular arc joining the ends of such a diameter. The line representing a rotation plane is a full line which is labelled with a 3, 4 or 6 to show its order, or left unlabelled if it is of order two.

If the rotation plane contains the *z* axis then it is represented by a diameter of the primitive* and its effect in the hyperstereogram is to produce an ordinary rotation about this line. This was illustrated in paper I (for example No. 12, 5/01, class 22) for

* This assumes the convention always adopted here that the projection is made to project the *z* axis to the centre of the hyperstereogram.

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the case of twofold rotations, and its extension to higher orders is trivial and is not illustrated further here.

If the rotation plane is orthogonal to the z axis, then it is represented by a great circle of the primitive, and its effect is to produce a kind of toroidal rotation round this great circle (Whittaker, 1973*a*). To consider the representation of the effect on any particular point, a central section of the hyperstereogram is taken through the point, perpendicular to the great circle. This section is then exactly equivalent to an ordinary stereogram having a rotation axis represented at a point on the primitive. A twofold plane was exemplified in this situation in paper I, No. 6, 3/01, class 2. One is familiar with ordinary stereograms having twofold and fourfold axes represented on the primitive, but threefold and sixfold axes are less familiar in this situation. Fig. 2(*a*) shows a fourfold plane represented by the equator. Fig. 2(*b*) shows a sixfold plane in the same way, and its effect may be understood by comparison with that of the fourfold plane. Successive **6** operations transform the point marked *A* to the points *B*, *C*, *D*, *E* and *F*. A threefold plane is not illustrated, but its effect is easily understood as generating only alternate ones of the six points in Fig. 2(*b*), for example *A*, *C* and *E*.

A sixfold plane in a general position is shown in Fig. 3. The points are repeated round a circle on a plane orthogonal to the arc, the centre of the circle being somewhat outside the arc. As the plane containing the points is not a central section of the hyperstereogram the construction cannot so easily be related to an ordinary stereogram, but its nature can be seen to be intermediate between the cases when the rotation plane is represented by a diameter and a great circle. Rotation planes of other orders are entirely analogous. However, two new features arise in this case.

(i) If a point is sufficiently distant from the rotation plane some of its repetitions may lie outside the primitive, and when these are replotted as negative points inside they will spoil somewhat the circular arrangement of points. This problem occurs equally in ordinary stereograms that contain rotation axes not at z and not on the primitive.

(ii) The full line only represents half of the rotation plane, the other half lying outside the primitive. This is replotted as a negative (broken) arc inside the primitive, and this negative half will rotate any negative points in the hyperstereogram in exactly the same way as the positive half rotates positive points. Positive points are not rotated round the negative half nor are negative points rotated round the positive half.

Axes of rotation–inversion

The representation of $\bar{1}$ axes was discussed and illustrated in paper I. In the case of higher-order axes it is necessary to show the orientation of the component rotation plane as well as the point representing the direction of the rotation–inversion axis. The former is symbolized by a chain line instead of a full line, and the latter by means of the conventional symbols △, □, ⬡ threaded on the line and with their own plane orthogonal to it. An example of a $\bar{4}$ axis is shown in Fig. 4. If the four symmetry-related points are close to the axis the $\bar{4}$ symmetry is very obvious; if they are somewhat distant from it, it is necessary to remember that they move outward from the virtual 4 plane on spherical caps so that the further they are from the $\bar{4}$ axis in Fig. 4 the closer they are to the *xyz* plane.

Fig. 5 shows an example of a $\bar{3}$ axis, and it is clear from this that the $\bar{3}$ axis is equivalent to a combination of an explicit $\bar{1}$ axis and an explicit 3 plane (*cf.* the $\bar{\mathbf{3}}$ operation in three dimensions). It is therefore usually more convenient to show the component rotation plane by a full line. Similarly, a $\bar{6}$ axis (Fig. 6) is equivalent to a combination of a 3 plane and a perpendicular m hyperplane, and again it is usually more informative to indicate it by means of a full line (marked 3) than a chain line (marked 6).

Point symmetry elements

Double rotations involving a 2 plane

Reasons were given in paper I for using unitary symbols for these operations, namely $\bar{\bar{\mathbf{1}}}$, $\bar{\bar{\mathbf{3}}}$, $\bar{\bar{\mathbf{4}}}$ and $\bar{\bar{\mathbf{6}}}$ for **22**, **62**, **42** and **32** respectively. The nature of $\bar{\bar{\mathbf{1}}}$ was illustrated by the hyperstereogram of No. 2, 1/02, class $\bar{1}$, and it was pointed out that it is not possible to locate any geometrical symbol for point symmetry elements in the hyperstereogram. In what follows their presence is indicated where necessary by a symbol below the hyperstereogram. For the symmetry element $\bar{\bar{1}}$ the symbol used is $\bar{\bar{1}}$ itself.

Fig. 7 illustrates $\bar{\bar{\mathbf{3}}}$, $\bar{\bar{\mathbf{4}}}$ and $\bar{\bar{\mathbf{6}}}$. It will be seen (and may of course be verified by matrix algebra) that a $\bar{\bar{3}}$ point involves an explicit 3 plane combined with a $\bar{\bar{1}}$ point, and it is most informative to symbolize it in this way. $\bar{\bar{\mathbf{4}}}$ does not involve an explicit rotation plane or a $\bar{\bar{1}}$ point, and its component virtual 4 plane is therefore shown by a chain line. It is distinguished from $\bar{4}$ by the absence of any symbol threaded on it. $\bar{\bar{\mathbf{6}}}$ is shown similarly in Fig. 7(*c*), though it may also be shown by an explicit 3 plane together with an explicit orthogonal 2 plane (in this case on *yz*) corresponding to its formulation as a double rotation **32**, and it is easiest to understand the operation in these terms.

Double rotations of equal orders

Fig. 8 shows the effect of a particular example of what has hitherto been called the double rotation **44**.

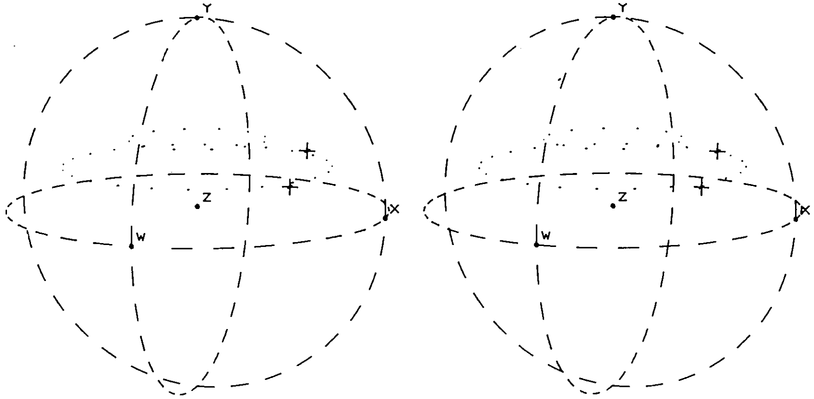


Fig. 1. A mirror hyperplane represented by an inverted saucer-shaped spherical cap intersecting the primitive in the equator.

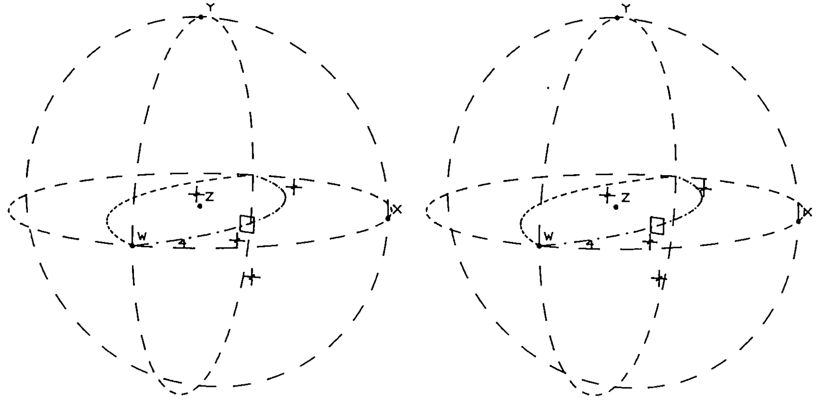


Fig. 4. A $\bar{4}$ axis in a general orientation represented by □. Its component virtual 4 plane is represented by the chain line · — · — · —.

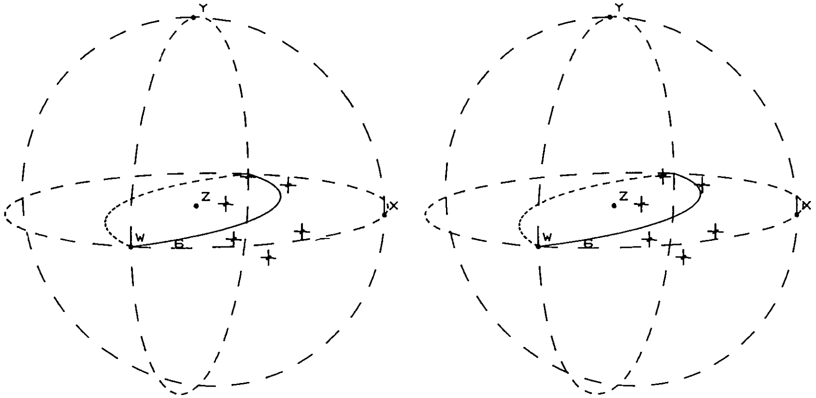


Fig. 3. A sixfold rotation plane in a general orientation. The arc consisting of short dashes represents its negative extension re-projected to the north pole of the hypersphere so as to lie inside the primitive.

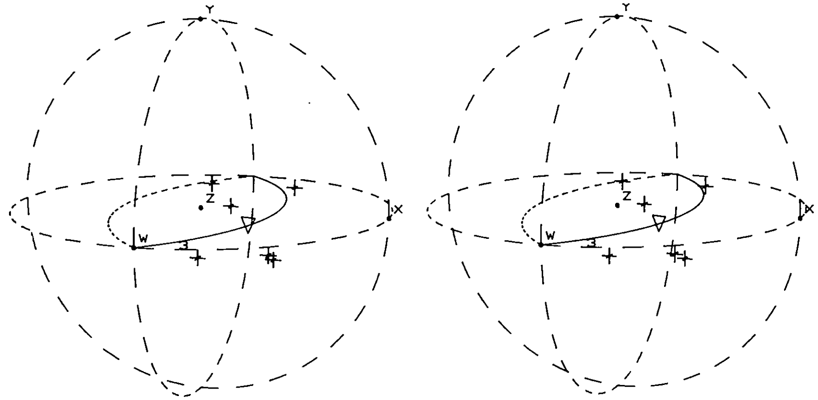


Fig. 5. A $\bar{3}$ axis in a general position. Its component 3 plane is explicitly present and is shown by the full line. Its component $\bar{1}$ axis is coincident with the $\bar{3}$ axis and is not shown separately.

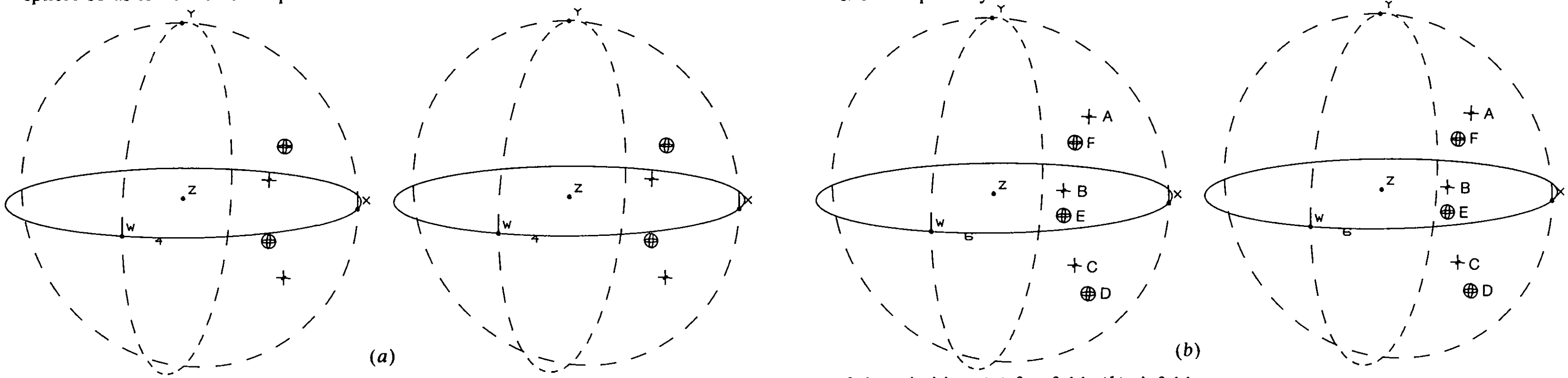


Fig. 2. Rotation planes represented by the equator of the primitive: (a) fourfold; (b) sixfold.

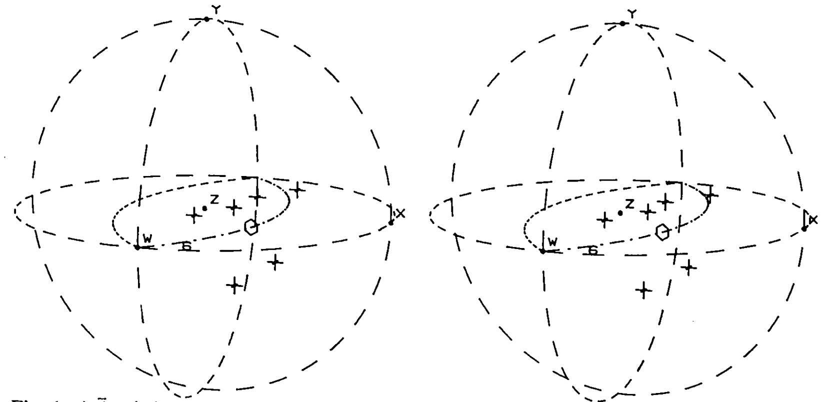


Fig. 6. A $\bar{6}$ axis in a general position. The component virtual 6 plane is shown by a chain line, but an explicit 3 plane coincides with it and there is an explicit m hyperplane (not shown) perpendicular to it at the position of the $\bar{6}$ axis.

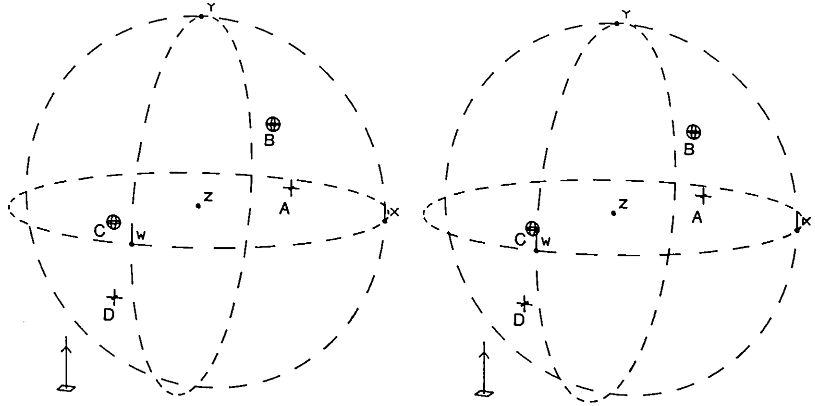


Fig. 8. A IV point.

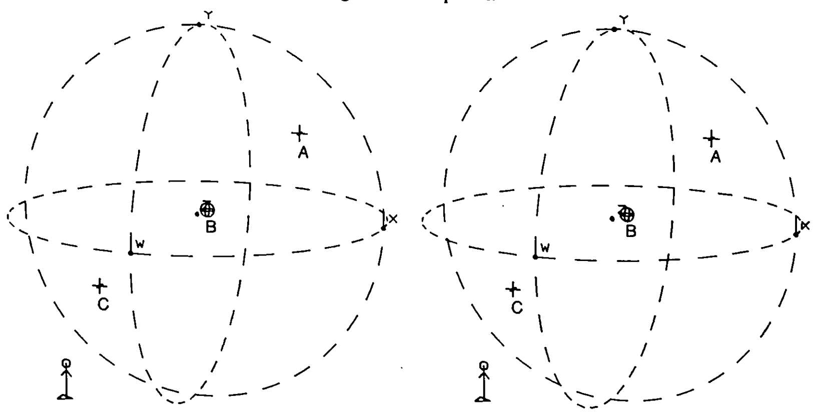


Fig. 9. A III point.

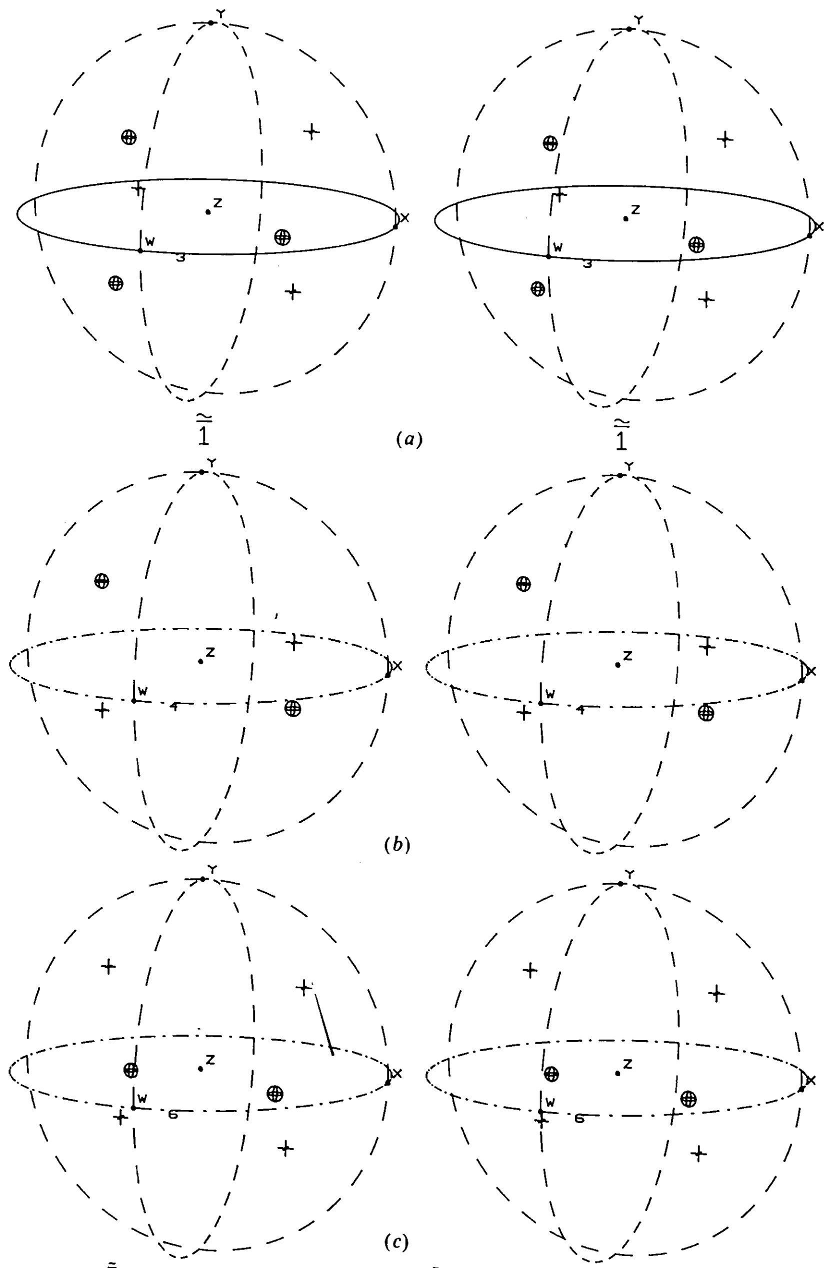


Fig. 7. (*a*) $\bar{\bar{3}}$ shown by its explicit 3 plane and $\bar{\bar{1}}$ point; (*b*) $\bar{\bar{4}}$ shown by the chain line on its component virtual 4 plane; (*c*) $\bar{\bar{6}}$ shown by the chain line on its component virtual 6 plane.

It can be understood as the combined operation of a 90° rotation about *wx* with a 90° rotation about *yz*, and its matrix representation can be factorized into the matrices of these two **4** operations as

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

It would be inappropriate, however, to label *wx* and *yz* as constituent virtual 4 planes because they have no unique status. The matrix can in fact be factorized into the product of the **4** operation

$$\frac{1}{2}\begin{pmatrix} 1-\cos p\cos q & -1-\cos p\cos q & \begin{matrix}\sin p \\ -\cos p\sin q\end{matrix} & \begin{matrix}\sin p \\ +\cos p\sin q\end{matrix} \\ 1+\cos p\cos q & 1-\cos p\cos q & \begin{matrix}-\sin p \\ -\cos p\sin q\end{matrix} & \begin{matrix}\sin p \\ -\cos p\sin q\end{matrix} \\ \begin{matrix}\sin p \\ +\cos p\sin q\end{matrix} & \begin{matrix}-\sin p \\ +\cos p\cos q\end{matrix} & -1-\cos p\cos q & 1-\cos p\cos q \\ \begin{matrix}\sin p \\ -\cos p\sin q\end{matrix} & \begin{matrix}-\sin p \\ -\cos p\cos q\end{matrix} & -1+\cos p\cos q & -1-\cos p\cos q \end{pmatrix}$$

and an orthogonal **4** operation, where *p* and *q* are freely variable parameters. Thus there are no uniquely identifiable **4** components in the double rotation, which strongly reinforces the desirability of a unitary symbol. The symbol **IV** is therefore adopted for this purpose. Since the orientation of a plane in four dimensions requires four parameters for its specification, and two of these (which can be identified as *p* and *q* in the above matrix) have no effect on the resultant **IV** operation, the latter has an orientation requiring two parameters to specify it. The geometrical symbol shown at the bottom left of Fig. 8 uses the square to symbolize the fourfold character. If the centre of the square is taken as the position of the *z* axis in a small-scale hyperstereogram, then a line joins this to the point to which the *z* axis is transformed by the **IV** operation concerned. In Fig. 8 this is the *y* axis. A convention has to be adopted that it is always shown as a direction with a positive or zero *y* component. This is always possible, since if a given **IV** operation transforms *z* to $\bar{y}$, one represents the corresponding $\mathbf{IV}^3$ operation which transforms *z* to *y*. Thus the orientation of the line represents the two orientation parameters of the **IV** operation. In addition, it is necessary to specify the relative hand of the two component virtual **4** operations. This is done by an arrow outwards from *z* if the **IV** operation transforms an axis orthogonal to the line by a 90° rotation corresponding to a right-handed outward screw from *z* along the line. An inward pointing arrow indicates that the rotation is left-handed. The orientation of the symbol and the arrow then provides sufficient information to define the matrix of the **IV** operation.

It becomes relevant at this stage to discuss a question of nomenclature. The definition of a symmetry element is the geometrical locus of points that are invariant under the symmetry operation **M**. When the symmetry element is a plane its orientation and order label (*n*) define the whole group of symmetry operations $\mathbf{M}, \mathbf{M}^2 \ldots \mathbf{M}^n$. The same is true for an *m* hyperplane and for an axis of rotation–inversion, and the term symmetry element is commonly used both in the strictly geometrical sense and also in this derivative sense. With the introduction of a graphical symbol for the order and orientational characteristics of the **IV** operation it becomes possible to extend this usage to the 'IV symmetry element'. Although geometrically this is only the point (0, 0, 0, 0), its association with the orientational symbol makes this convenient usage meaningful, and it will become equally applicable to the other point symmetry elements in the following discussion.

In Fig. 8 successive applications of the specified **IV** operation transform the point marked *A* to *B*, *C*, and *D*. It is evident from the relationship of *A* to *C* and *B* to *D* that $\mathbf{IV}^2 = \bar{\mathbf{1}}$.

Entirely similar considerations apply to the double rotation **33**. It is therefore denoted **III**, and its effect and appropriate graphical symbols are shown in Fig. 9. The double rotation $\bar{\mathbf{6}}\mathbf{6}$ is equivalent to a combination of explicit **III** and $\bar{\mathbf{1}}$ operations, and it is therefore denoted $\mathbf{I\bar{I}I}$ and symbolized by the III and $\bar{1}$ symbols in Fig. 10, in which successive applications of the $\mathbf{I\bar{I}I}$ operation transform the point marked *A* to the points *B*, *C*, *D*, *E* and *F*. It may be observed that the points *A*, *E*, *C* are identical with points *A*, *B*, *C* (respectively) of Fig. 9, corresponding to the relationship $\mathbf{I\bar{I}I}^4 = \mathbf{III}$. Also, it is evident from the relationships of points *A* to *D*, *B* to *E* and *C* to *F* that $\mathbf{I\bar{I}I}^3 = \bar{\mathbf{1}}$.

Double rotations of unequal orders (greater than two)

The double rotation **63** may be factorized as

$$\mathbf{63 = 6.3 = 2.3.3 = 2.III}.$$

In the third of these forms the symmetry element of the **2** operation and the first **3** operation are a 2 plane and a coincident 3 plane. However, because of the two free parameters involved in the **III** operation (similar to *p* and *q* in the previous section) the **III** may be re-factorized to give component **3** operations, neither of which has its symmetry element coincident with the 2 plane. Thus, the '**63**' operation can be derived from certain combinations of a **2** and two **3** operations that do not include any **6** operation. It is most appropriately designated **VI**, and symbolized graphically as in Fig. 11 by a combination of the appropriate III symbol and 2 plane which correspond to $\mathbf{VI}^4$ and $\mathbf{VI}^3$ in the required orientation. The relationship $\mathbf{VI}^4 = \mathbf{III}$ may be recognized from the identity of the points *A*, *E*, *C* in Fig. 11 with the points *A*, *B*, *C* of Fig. 9, while the relationship $\mathbf{VI}^3 = \mathbf{2}$ is obvious from the pairs of points *AD*, *BE* and *CF*.

The double rotation **34**, which is a twelvefold operation, is denoted **XII** as an extension of the nomenclature. It has the properties $\mathbf{XII}^3 = \mathbf{4}^3$ and $\mathbf{XII}^4 = \mathbf{3}$ and these rotation operations have the same 4-plane and 3-plane symmetry elements as the operations that are combined to give **XII**. It is accordingly indicated fully by the representation of these two rotation planes as full lines, as shown in Fig. 12. Successive applications of the **XII** operations lead to the sequence *A*, *B*, *C*, . . . , *L*, while applications of the constituent **3** and **4** operations move along the series by four steps and nine steps at a time, respectively.

The double rotation **64** may be expressed as

$$\mathbf{64} = \mathbf{2.3.2.4}^3 = \mathbf{22.34}^3 = \tilde{\bar{\mathbf{1}}}.\mathbf{XII}^7.$$

It is therefore denoted by $\mathbf{X\tilde{\bar{I}}I}$. It has the properties $\mathbf{X\tilde{\bar{I}}I}^3 = \tilde{\bar{\mathbf{4}}}^3$ and $\mathbf{X\tilde{\bar{I}}I}^4 = \mathbf{3}$, and is therefore represented as in Fig. 13. Again the individual **3** and $\tilde{\bar{\mathbf{4}}}$ transform the points in such a way as to move four steps and nine steps, respectively, along the alphabetic sequence.

Multiple rotations

Of the two symmetry operations in this category the easier one to deal with is **3344**. It is another twelvefold operation, and for lack of a better symbol is denoted **XII′**. It has the properties $\mathbf{XII}'^3 = \mathbf{IV}^3$ and $\mathbf{XII}'^4 = \mathbf{III}$ and these are the component double rotations from which it is constructed. It is therefore represented by symbols for both of them, as in Fig. 14. In the particular example illustrated the IV and III symbols are at right angles to one another to make it easier to follow their effects, but they could in fact be at any angle. The effect of the component **IV** operation may be followed by moving nine steps at a time along the alphabetical cycle: *A*, *J*, *G*, *D* correspond to *A*, *B*, *C*, *D*, respectively, in Fig. 8. The sequence *A*, *E*, *I* generated by successive applications of the **III** operation is more difficult to compare with Fig. 9 because of its different orientation and opposite hand.

The triple rotation **444** presents more difficulties. It is eightfold, and if it is denoted **VIII** it has the properties $\mathbf{VIII}^2 = \mathbf{IV}$ and $\mathbf{VIII}^4 = \tilde{\bar{\mathbf{1}}}$. The three component **4** operations are not all related to one another in the same way. Two of them form an orthogonal pair that generate a **IV** operation, but the third is necessarily nonorthogonal to either of them, though it has to be in a specific orientation relative to this **IV** operation. Thus one can factorize **VIII** as **4.IV**, but these factors are not unique; that is, differently oriented **IV** operations can be combined with appropriate **4** operations to generate one and the same **VIII**. Moreover, the **IV** operation that is the square of **VIII** cannot be employed in generating it. There is thus no possibility of using the symbols of the components as has been done for **VI**, **XII**, $\mathbf{X\tilde{\bar{I}}I}$ and **XII′**. The graphical symbol adopted is shown (for a particular orientation) in Fig. 15. Since the eight powers of **VIII** form a group, one may without loss of generality choose any of the odd powers as the fundamental one. There are two of these odd powers whose squares transform *z* to a possible orthogonal axis and satisfy the convention adopted for deriving the symbol of a **IV** operation, and the symbol of this is used as a basis. Two lines are added to this symbol to show the two successive **VIII** transformations that lead to the symbolized **IV** operation.

In order that the VIII symbol should uniquely define the matrix of the **VIII** operation involved it is necessary to specify a further convention. In crystal systems 26 and 32 the **VIII** operation (when present) relates the eight $\pm w$, $\pm x$, $\pm y$, $\pm z$ crystallographic axes. For the purpose of constructing the symbol the fundamental member of the group formed by the powers of **VIII** must be taken as that one of the two already chosen which transforms *z* to a positive axial direction. In Fig. 15 this is *x*, and for the sake of simplicity is shown as orthogonal to *z*, although this condition is not imposed by the **VIII** operation and does not exist in system 26. In system 33 **VIII** operations occur which lead to transformations such as $z \rightarrow [1111] \rightarrow y$, and in this case a different convention would be necessary that would lead to an acute angle between the initial line and the direction of the IV symbol. However, symbols for VIII symmetry elements are in fact never needed in system 33 because the **VIII** operations always arise implicitly from combinations of simpler symmetry operations.

In Fig. 15 it may readily be observed that the sequence of points *A*, *C*, *E*, *G* is identical with *A*, *B*, *C*, *D* of Fig. 8, corresponding to the relationship $\mathbf{VI\tilde{\bar{I}}I}^2 = \mathbf{IV}$.

The fivefold and tenfold operations

It has previously been shown that the fivefold operation (denoted **V** to distinguish it from a non-crystallographic fivefold rotation) can be regarded as a combination of a $\bar{\mathbf{4}}$ operation with an **m** operation in a particular relationship to one another (Whittaker, 1973*b*). However, this is not very helpful in visualising its effect. The operation has the property that there exist five directions in four-dimensional space (represented by five points in the hyperstereogram of which no set of four are coplanar) which are transformed cyclically into one another. Four of these directions may be chosen as (non-orthogonal) axes, and the fifth is then the direction $[\bar{1}\bar{1}\bar{1}\bar{1}]$. It is always possible to choose as fundamental that member of the group constituted by the five powers of **V** which transforms *z* to *y*. The projections of the axes *w*, *x*, *y* and $[\bar{1}\bar{1}\bar{1}\bar{1}]$ surround the projection of *z* tetrahedrally (the tetrahedron may be regular or may have two

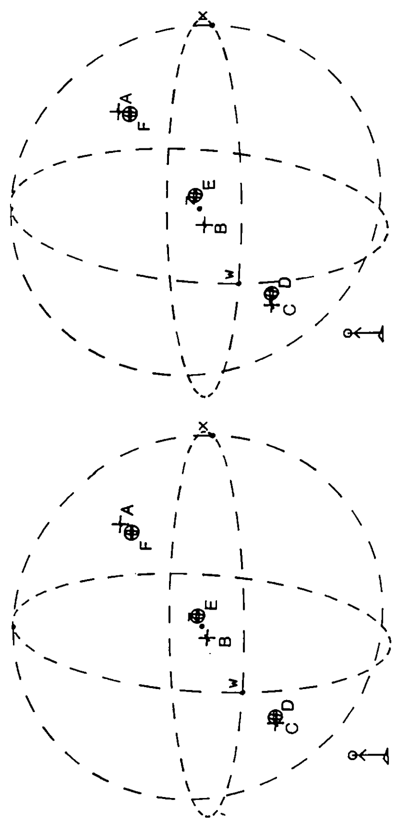


Fig. 10. A $I\bar{\bar{I}}I$ point shown by its component III point and a $\bar{\bar{1}}$ point which are explicitly present.

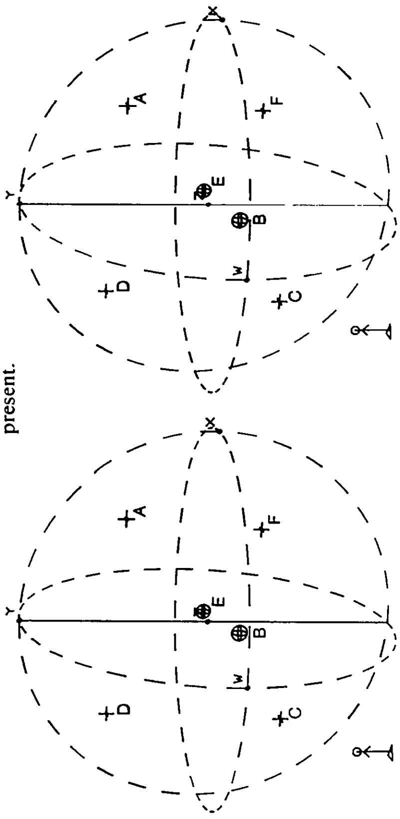


Fig. 11. A VI point shown by its component 2 plane and III point which are explicitly present.

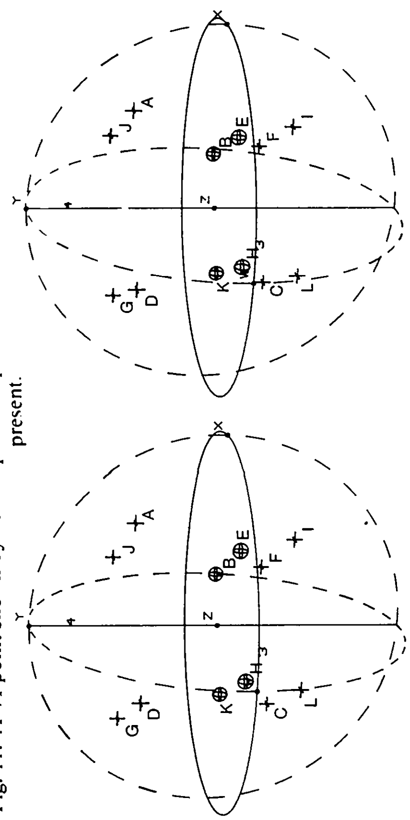


Fig. 12. A XII point shown by its component 4 plane and 3 plane which are explicitly present.

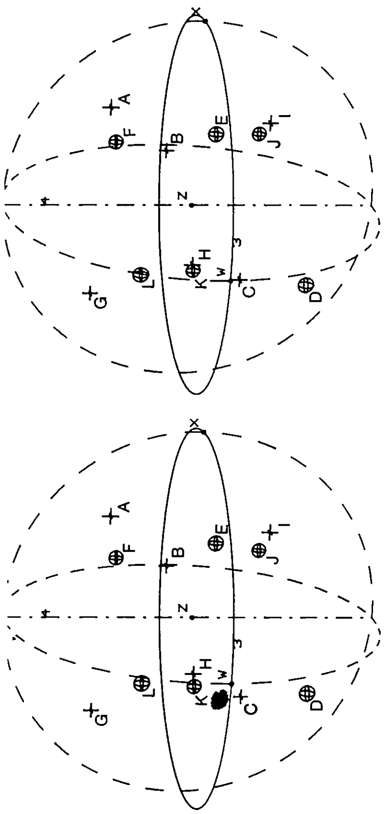


Fig. 13. A $X\bar{\bar{I}}I$ point shown by its component $\bar{\bar{4}}$ point and 3 plane which are explicitly present.

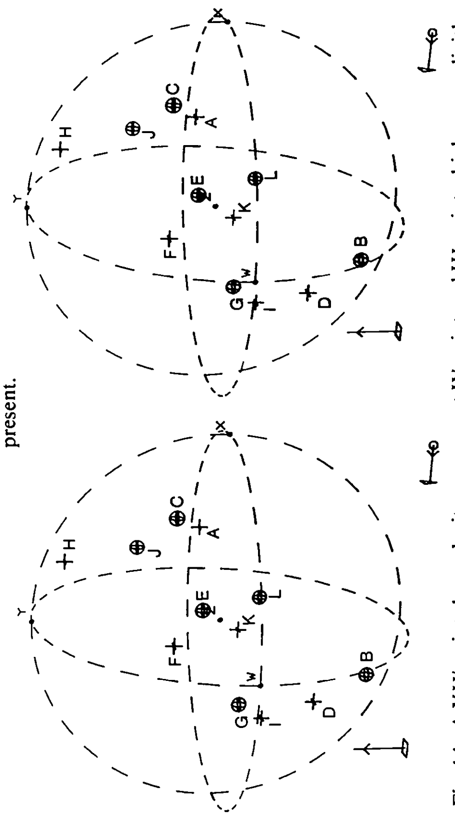


Fig. 14. A XII′ point shown by its component IV point and III point which are explicitly present.

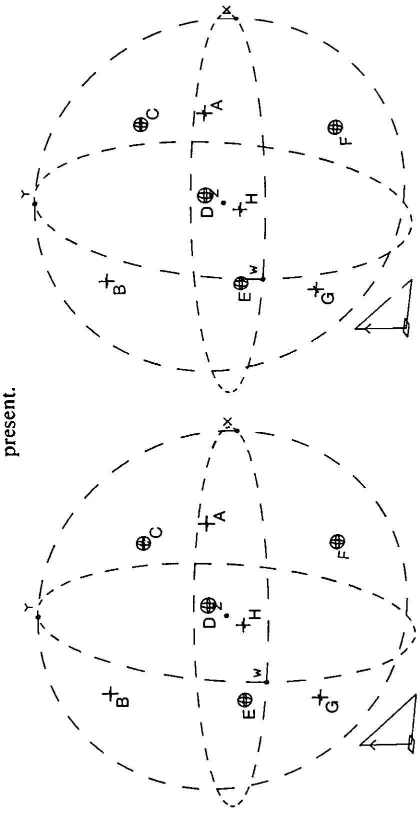
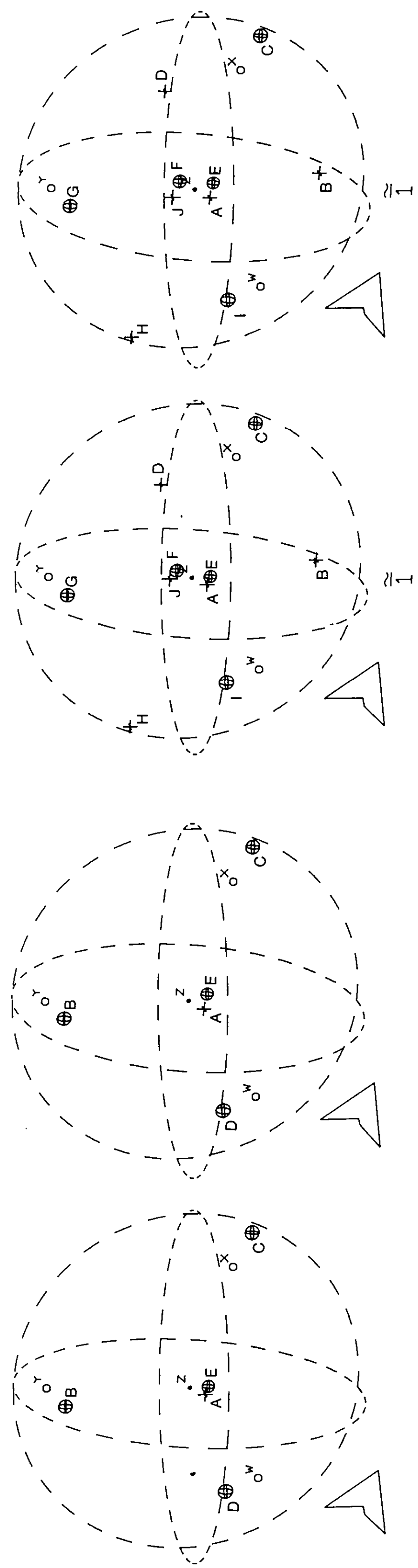


Fig. 15. An VIII point.



(a) (b)

Fig. 16. (a) A V point; (b) a $\bar{\bar{\mathbf{V}}}$ point shown by its constituent V point and $\bar{\bar{1}}$ point which are explicitly present.

unequal sets of three equal edges) and the route taken by z through y and then *via* one of the six possible permutations of w, x, $[\bar{1}\bar{1}\bar{1}\bar{1}]$ back to z can be depicted by joining up these points in the appropriate order. An example is shown in Fig. 16(*a*). In some crystal classes all six **V** operations are present together and the symbol then takes the form of a complete tetrahedron with all four vertices joined to its centre.

In Fig. 16(*a*) the points repeated by the symmetry have been chosen to lie close to the axes so that one can see the relationship between their pattern of repetition and that of the axes. It is to be noted that whereas the six different versions of the **V** operation that correspond to a particular set of axes simply cycle the axes in different orders but into the same places, they cycle an off-axis point to different points in the vicinity of the other axes.

The effect of the tenfold operation is illustrated in Fig. 16(*b*). It may be seen that it is equivalent to Fig. 16(*a*) but with every point accompanied by an opposite point of opposite sign. Thus the tenfold operation is equivalent to $\mathbf{V}.\bar{\bar{\mathbf{1}}}$. It is therefore denoted $\bar{\bar{\mathbf{V}}}$ and is represented by the V and $\bar{\bar{1}}$ graphical symbols. The relationship $\bar{\bar{\mathbf{V}}}^2 = \mathbf{V}^2$ is demonstrated by the identity of the points A, C, E, G, I in Fig. 16(*b*) with the points A, C, E, B, D, respectively, of Fig. 16(*a*), and the relationship $\bar{\bar{\mathbf{V}}}^5 = \bar{\bar{\mathbf{1}}}$ is evident from the pairs of points AF, BG, CH, DI and EJ.

Conclusions

The nature and orientational dependence of the four-dimensional crystallographic symmetry operations have been clarified by representing their effects by means of the hyperstereogram. Unitary symbols have been devised for all the double and multiple rotation operations, and the correspondences between the old and new symbols are summarized as follows:

22, 62, 42 and **32**	become $\bar{\bar{\mathbf{1}}}$, $\bar{\bar{\mathbf{3}}}$, $\bar{\bar{\mathbf{4}}}$ and $\bar{\bar{\mathbf{6}}}$, respectively;
33, 66 and **44**	become **III**, $\mathbf{I\bar{\bar{I}}I}$ and **IV**, respectively;
36, 34 and **64**	become **VI**, **XII** and $\mathbf{X\bar{\bar{I}}I}$, respectively;
444 and **3344**	become **VIII** and **XII′**, respectively.

The operations previously denoted **V** and **X** (Whittaker, 1973*b*) become **V** and $\bar{\bar{\mathbf{V}}}$. This clarification, and the availability of a suitable notation, are necessary pre-requisites for the development of a Hermann–Mauguin type of nomenclature for the crystal classes, and this will form the subject of paper III of this series. A sufficient set of graphical symbols has also been derived to denote all types of symmetry elements and their orientations on hyperstereograms, and this is a necessary pre-requisite for the preparation of an atlas of hyperstereograms of the 227 crystal classes, to be published elsewhere (Whittaker, 1984).

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SHORT COMMUNICATIONS

Contributions intended for publication under this heading should be expressly so marked; they should not exceed about 1000 *words; they should be forwarded in the usual way to the appropriate Co-editor; they will be published as speedily as possible.*

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Karle–Hauptman determinants and entropy.

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Abstract

That positivity of all the Karle–Hauptman determinants and the positivity of the electron density in the unit cell are equivalent conditions is well known. A simple way of deriving this result is presented providing at the same time a relation between these determinants and the logarithm of the electron density. The relationship of this logarithm of the electron density to the entropy is also discussed.

The Karle–Hauptman determinants are determinants of matrices involving the structure factors $F_{\mathbf{H}}$ (Karle & Hauptman 1950),

$$F_{\mathbf{H}} = (1/V)\int \rho(\mathbf{r}) \exp(2\pi i \mathbf{H}\mathbf{r})\, \mathrm{d}r.$$

The structure factors are arranged into a matrix by writing $\mathbf{H} = h_1\mathbf{b}_1 + h_2\mathbf{b}_2 + h_3\mathbf{b}_3$, where $\mathbf{b}_i$ are the reciprocal-lattice vectors, and by grouping the three indices h_1, h_2, h_3 into one, 'm', by writing

$$m = h_1 + N(h_2 - 1) + N^2(h_3 - 1), \qquad (1)$$

where $(N-1)$ is the maximum value of h_i to be included in the matrix. A matrix D^N of order N^3 with elements

$$D^N_{mn} = F_{m-n}, \quad m, n = 1, \ldots, N^3$$

can now be formed. The Karle–Hauptman determinants up to order N^3 are all the principal minors of D^N, including $\det(D^N)$ and are positive if and only if $\rho(\mathbf{r}) > 0$.

Narayan & Nityananda (1982) showed that:

$$\lim_{N\to\infty} (1/N^3) \log[\det(D^N)] \to (1/V) \int \log \rho(\mathbf{r})\, \mathrm{d}r. \qquad (2)$$

Both of these results will be recovered together with some other results.

For the derivation, the unit cell is considered to be divided into N^3 pixels, N divisions along each space direction, with integers j_1, j_2, j_3 specifying a pixel. As shown in the Appendix there exist values $\bar{\rho}_{\mathbf{j}}$ such that

$$F_{\mathbf{h}} = (1/N^3) \sum_{\mathbf{i}}^{N} \bar{\rho}_{\mathbf{j}} \exp(2\pi i \mathbf{j}\mathbf{h}/N),$$

with $\bar{\rho}_{\mathbf{j}}$ a sampled value of the electron density $\rho(\mathbf{r})$ in pixel $\mathbf{j}$. In the same way as for the structure factors, the indices $\mathbf{j}$ are arranged into one, κ, by the same type of formula as (1).

The numbers $\bar{\rho}_\kappa$ are now considered to be the diagonal elements of a diagonal matrix B, *i.e.* B has elements $B_{\mu\kappa} = \rho_\kappa \delta_{\mu\kappa}$, with $\delta_{\mu\kappa}$ the Kronecker delta. By a unitary transformation R the matrix B is transformed into D^N as follows: Let the matrix R have elements $R_{\kappa n} = (1/N^{3/2}) \exp(2\pi i \mathbf{j}\mathbf{h}/N)$, with κ related to $\mathbf{j}$ and n to $\mathbf{h}$ *via* (1), and let R^* denote the Hermitian conjugate of R, then it is easy to show that R is unitary, *i.e.* $R^*R = I$, I the identity matrix, and that

$$D^N = R^*BR.$$

It is here understood that in the matrix multiplication the summation over, say, κ, related to $\mathbf{h}$ *via* (1), from 1 to N^3 is really a sum over h_1, h_2 and h_3, each from 1 to N. It is obvious that $\rho_1, \ldots, \rho_N$ are the eigenvalues of the matrix D^N. The results now follow by the following theorems (Wilkinson, 1965).

(*a*) A necessary and sufficient condition for a Hermitian matrix to be positive definite is that all its eigenvalues are positive.

(*b*) A necessary and sufficient condition for a Hermitian matrix to be positive definite is that all its principal minors are positive.

In essence then, if $\rho(\mathbf{r}) > 0$ then by (*a*) D^N is positive definite and by (*b*) all the principal minors (Karle–

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