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Graphic Representation and Nomenclature of the Four-Dimensional Crystal Classes. I. Classes with Symmetry Operations of Order Not Greater Than Two

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Abstract

Hyperstereographic projections have been prepared (in the form of stereo-pairs) of the sixteen four-dimensional (geometric) crystal classes that contain only symmetry operations of order not greater than 2. These provide an initial demonstration of the usefulness of the hyperstereographic projection in visualizing the nature of four-dimensional symmetry elements and symmetry groups. The clarification thus introduced into the subject has suggested a rationalized system of symbolic nomenclature following the general principles of the Hermann–Mauguin notation.

Introduction

The symmetry of all the 227 four-dimensional geometric crystal classes (here abbreviated to crystal classes) has been tabulated by Brown, Bülow, Neubüser, Wondratschek & Zassenhaus (1978) as part of their work on the crystallographic space groups of four-dimensional space. However, the form of this tabulation in terms of generating matrices is not conducive to a ready visualization of the symmetries involved and their relationship to those of the three-dimensional crystal classes. The latter are commonly illustrated by stereograms on which the symmetry elements are represented by a code of graphic symbols in their mutual orientations, and the symmetrical repetition of a point, in an arbitrary general position, is displayed. The same thing can be done for the four-dimensional case by using the hyperstereographic projection (Whittaker, 1973*a*). This is a three-dimensional figure, however, and is correspondingly more difficult to construct. A model was constructed (Whittaker, 1973*b*) to show the arrangement of the rotation planes in the symmetry of the hypercube (class 32/21 of the tabulation of Brown *et al.*, 1978). However, the work involved in building such models precludes their production for more than a very few crystal classes, and even then it would be difficult to include in them a set of symmetry-related points.

The problem has now been surmounted by the preparation, by computer graphics, of stereo-pairs of hyperstereograms. These not only illustrate the symmetry of each crystal class, but also illuminate in a graphic way the nature and relationship of the 33 crystal systems of four dimensions, and also the nature of the less-obvious symmetry operations of four-dimensional space. They also suggest a way of extending the Hermann–Mauguin nomenclature of crystal classes so as to deal with the complications introduced by a fourth dimension.

The illustrations in this paper are confined to the first 16 crystal classes. These belong to the first six crystal systems of Brown *et al.* (1978) and comprise all those which involve no symmetry operation of order greater than 2. The technique is by no means limited to these (and work is well advanced on the remaining 211), but they provide a sufficient sample to illustrate the power of the method.

Computation

The computation was done using the graphics package GINO-F on the Digital VAX 11/780 computer of the Oxford University Computing Service. The plots were produced in ink on a Calcomp 1051. The size of the stereograms plotted was limited to 10 cm diameter in order to avoid undue loss of line thickness on reduction $\times\frac{1}{2}$ to give a separation of 5·5 cm between stereo-pairs. Point perspective was used at an eye distance of 40 cm from the centre of the 10 cm diameter sphere, and the two viewing directions were separated by an angle of 2·9°. The figures in this paper have been further reduced to fit onto the journal pages.

The symmetric repetition of the general point was computer generated in each case from generating matrices listed by Brown *et al.* (1978). The positions of the symmetry elements to be represented had to be determined by inspection of the full set of matrices.

Symmetry elements and their nomenclature

The symmetry element corresponding to a symmetry operation is defined as the subspace in which every

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point is invariant for the operation. It increases by one in its dimensionality for every increase of one in the dimensionality of the space in which the operation is defined, and the relationship is evident from matrix representations of the symmetry operators in simple cases.

Mirror reflection

In one dimension this is the only symmetry operation* (apart from the identity), and its matrix representation is $(\bar{1})$. It changes the sign of the single coordinate that exists, and its symmetry element is the point that it leaves invariant. In two dimensions change of sign of one coordinate leaving the second unchanged is represented by

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

if the first coordinate is taken as the one that is reversed by the symmetry. The symmetry element is then a line coincident with the axis of the second coordinate. Extension to the next higher dimensions by addition of 1 on the diagonal then leads to

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

whose symmetry elements are respectively a plane and a hyperplane perpendicular to the first axis. In any number of dimensions the appropriate symbol is *m*.

Rotation

Rotation first becomes possible in two dimensions, when its symmetry element is a point. The matrix for two-fold rotation can be derived from that for one-dimensional reflection by extension of the diagonal with a '$\bar{1}$' to give

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

Again, as the dimensionality is extended corresponding operations are obtained if ones are added along the matrix diagonal, so that twofold rotations in three and four dimensions are represented by

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

Higher-order three, four and sixfold rotations are not discussed in this paper, but the appropriate two-dimensional matrix may be extended to higher dimensions in the same way. All these rotations have symmetry elements that are respectively a rotation axis and a rotation plane, and are symbolized by the same numerals 2, 3, 4, 6.

Rotation–inversion

Just as a new kind of symmetry operation (rotation) arises in two dimensions when a $\bar{1}$ is added to the diagonal of the one-dimensional reflection matrix, so a new kind of symmetry arises in three dimensions if a rotation matrix

$$\begin{pmatrix} a & b \\ c & d \end{pmatrix} \text{ is extended to give } \begin{pmatrix} a & b & 0 \\ c & d & 0 \\ 0 & 0 & \bar{1} \end{pmatrix}.$$

This corresponds to a combination of a rotation

$$r, \begin{pmatrix} a & b & 0 \\ c & d & 0 \\ 0 & 0 & 1 \end{pmatrix}, \text{ with reflection } \begin{pmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & \bar{1} \end{pmatrix}$$

in a perpendicular plane. This is an operation of rotation–reflection, symbolized as $\tilde{r}$. The symbol $\bar{r}$ has been adopted as the symbol for a rotation–inversion

$$\begin{pmatrix} \bar{a} & \bar{b} & 0 \\ \bar{c} & \bar{d} & 0 \\ 0 & 0 & \bar{1} \end{pmatrix},$$

the product of the rotation r with

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

Use of the rotation–inversion rather than rotation–reflection has two advantages. The first is that it promotes the centre of inversion

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

symbolized as $\bar{1}$, to the fundamental role it deserves (because it is the only operation which commutes with all translation groups) instead of regarding it as $\tilde{2}$. The latter symbol is confusing as it has no directionality, since the component twofold rotation and perpendicular mirror can be taken in any arbitrary direction. The second advantage is that it also interchanges the symbols $\bar{3} = \tilde{6}$ and $\bar{6} = \tilde{3}$ which has advantages in the nomenclature of the trigonal and hexagonal systems.

In previous work on four-dimensional symmetry there has been a tendency to revert to the terminology of rotation–reflection (Kuntsevich & Belov, 1968; Whittaker, 1973*b*). However, the present work reveals that there are substantial advantages in preserving the rotation–inversion nomenclature; it promotes clarity

* Symmetry operations of infinite repeating patterns, as well as noncrystallographic symmetry, are excluded from the discussion.

for the same reasons as in three dimensions, and also brings out the relationships between four-dimensional symmetry and the familiar aspects of three-dimensional symmetry.

Although it is traditional to speak of *axes* of rotation–inversion in three dimensions, this is misleading. The symmetry element that is invariant under these operations is a point, although in the case of $\bar{3}$, $\bar{4}$ and $\bar{6}$ it is necessary to specify the direction of the component rotation. When dimensionality is extended to four the symmetry element truly becomes an axis, so that, for example, one has a $\bar{1}$ axis as the symmetry element corresponding to the operation

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

In the case of $\bar{3}$, $\bar{4}$ and $\bar{6}$ axes it is necessary to specify the orientation of the component rotation plane. The direction of the axis necessarily lies in this plane.

Operations with point symmetry elements in four dimensions

These have no counterpart in three dimensions. The simplest is obtained by adding a diagonal -1 to be matrix for the centre of inversion to give

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

This has hitherto been regarded as a 'double rotation'; *i.e.* a twofold rotation about *wx* combined with a twofold rotation about *yz* (Kuntsevich & Belov, 1968), and symbolized as 22 (Whittaker, 1973*b*). However, the component rotations have no defined orientation. It is therefore proposed to treat it as a unitary operation symbolized (for obvious reasons) as $\tilde{\bar{1}}$. Symmetry operations represented by corresponding extensions of the matrices for $\bar{3}$, $\bar{4}$ and $\bar{6}$ can similarly be symbolized as $\tilde{\bar{3}}$, $\tilde{\bar{4}}$ and $\tilde{\bar{6}}$ instead of 32, 42 and 62, though it is of course necessary to specify the orientation of their constituent 3, 4, or 6 rotation plane. The nature of these and of the remaining ten symmetry operations with point symmetry elements will be made much clearer by subsequent publications of illustrative hyperstereograms. Only $\tilde{\bar{1}}$ is illustrated in the present work.

Representation of symmetry elements in the hyperstereogram

The mathematics of the hyperstereogram has been presented previously (Whittaker, 1973*a*).

The primitive is the surface of the sphere. This is represented by broken lines along three orthogonal great circles, unless any symmetry element is to be denoted on those circles when another appropriate line is shown.

Mirror hyperplanes are represented by spherical surfaces in the hyperstereogram: on the primitive, on diametral planes, or on saucer-shaped spherical caps (Whittaker, 1973*a*, Fig. 1). They are denoted by dotted circles lying on them. In the case of a mirror on the primitive these are vertical small circles at $1/\sqrt{2}$ from the origin, and the orthogonal great circles are also dotted unless rotation planes are denoted on them, in which case their appropriate symbolism takes precedence. In the case of a mirror on a diametral plane the dotted circle is of radius 0·5. Spherical caps do not occur in the present work.

Rotation planes are represented in the hyperstereogram by great circles and diameters of the primitive, and (in other cases than those treated here) by circular arcs joining the ends of such diameters (Whittaker, 1973*a*, Fig. 2). Twofold rotation is denoted by a full line. Higher orders are denoted by an additional symbol but do not occur in the present work.

Rotation–inversion axes are represented by points in the hyper-stereogram. They are denoted by open symbols (a circle for $\bar{1}$) corresponding to those used in ordinary stereograms. Their component rotation planes are denoted when necessary by $-\cdot-\cdot$, but this does not occur in the present work.

Point symmetry elements do not intersect the hypersphere and so have no location in the hyperstereogram.

Representation of crystallographic axes in the hyperstereogram

The *z* axis is projected to the centre of the primitive where it is denoted by a dot. In orthogonal systems the *w*, *x* and *y* axes project on the primitive, respectively at the front and right-hand side of the equator and at the north pole. They are always on the primitive if the angles *wz*, *xz*, *yz* are right angles. If such angles are acute the axis plots inside the primitive. If they are obtuse the axes would plot outside the primitive, but they are then reprojected to the opposite pole of the hypersphere and are denoted by very small circles inside the primitive in the usual way.

Symmetric repetition of a general point

A general point with a positive (orthogonal) *z* coordinate is represented by a triaxial cross, and one with a negative one (reprojected to the opposite pole of the hypersphere so as to fall inside the primitive) as a small empty sphere of the same size.

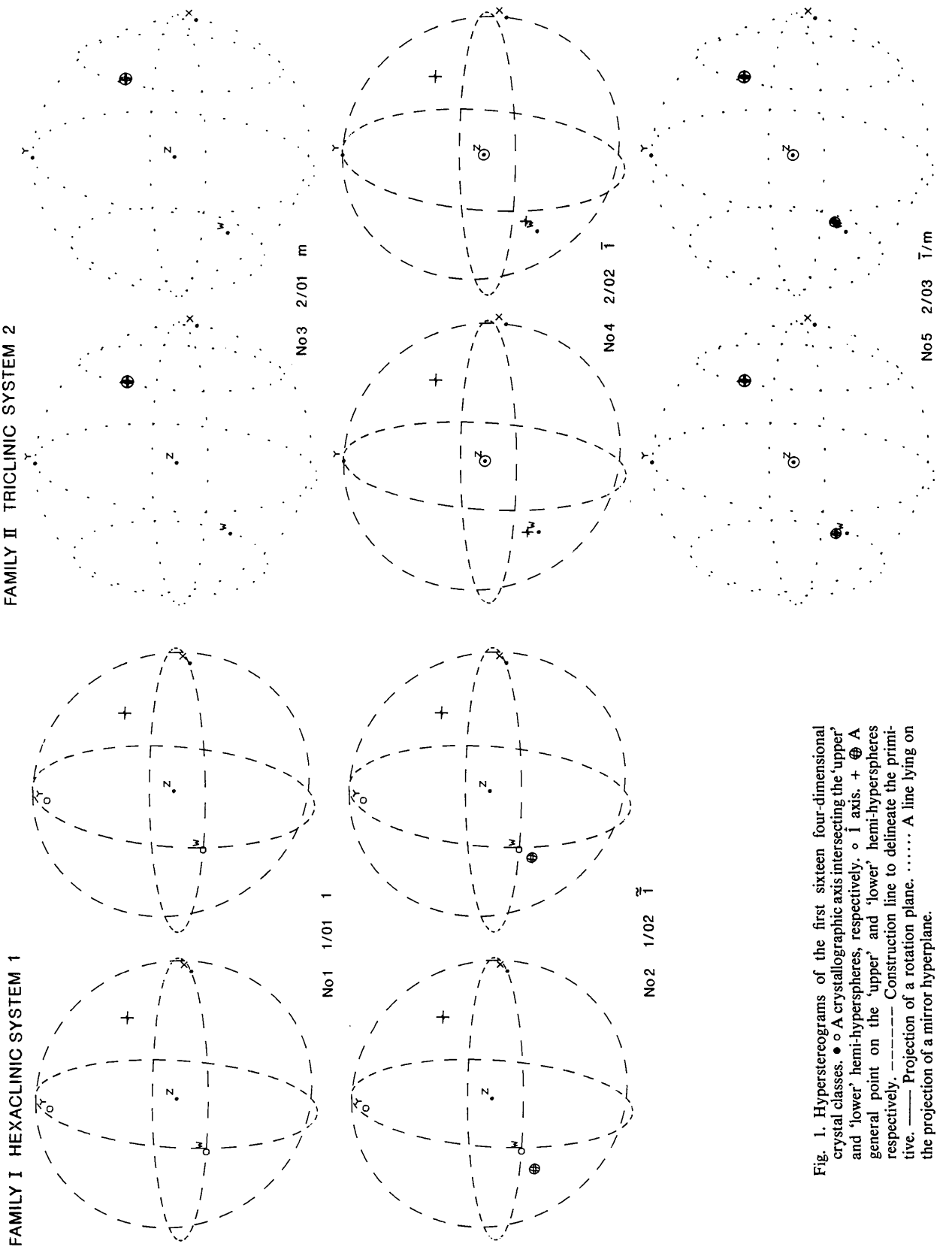
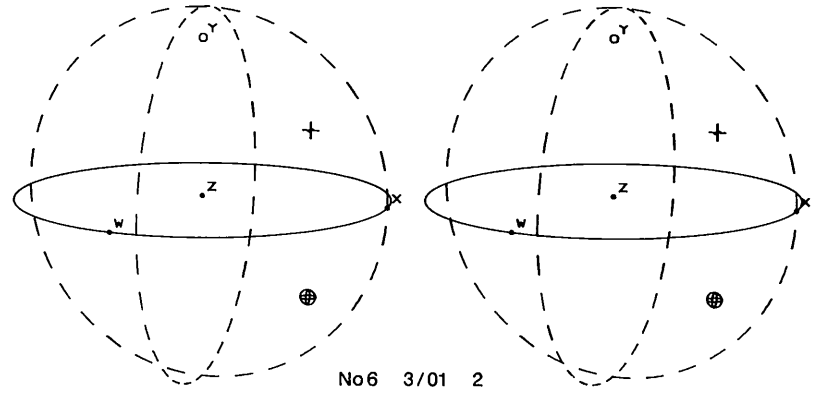
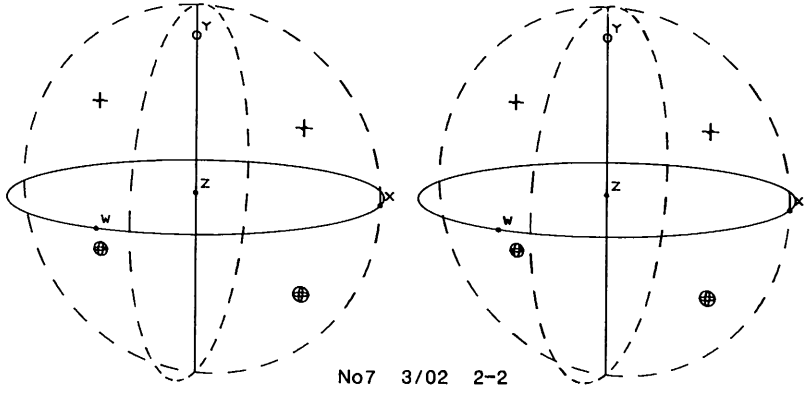


Fig. 1. Hyperstereograms of the first sixteen four-dimensional crystal classes. ● ○ A crystallographic axis intersecting the 'upper' and 'lower' hemi-hyperspheres, respectively. ○ $\bar{1}$ axis. + ⊕ A general point on the 'upper' and 'lower' hemi-hyperspheres respectively. – – – – – – Construction line to delineate the primitive. —— Projection of a rotation plane. ····· A line lying on the projection of a mirror hyperplane.

FAMILY III DICLINIC SYSTEM 3

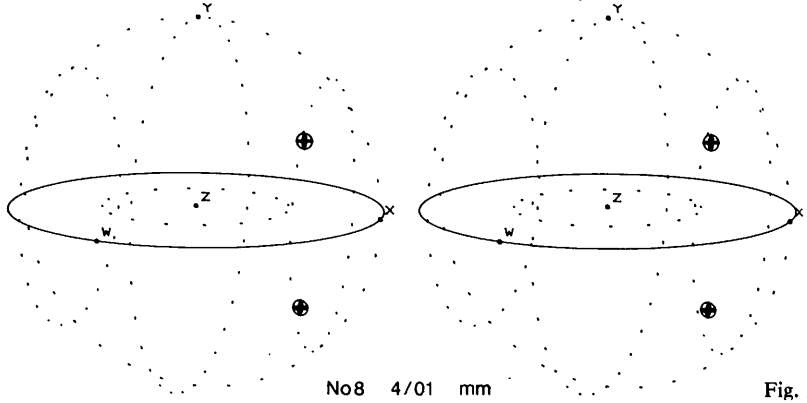


No6 3/01 2



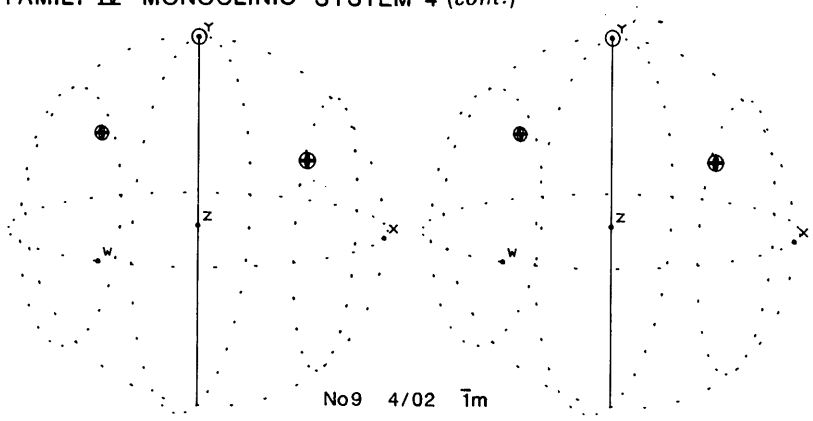
No7 3/02 2-2

FAMILY IV MONOCLINIC SYSTEM 4

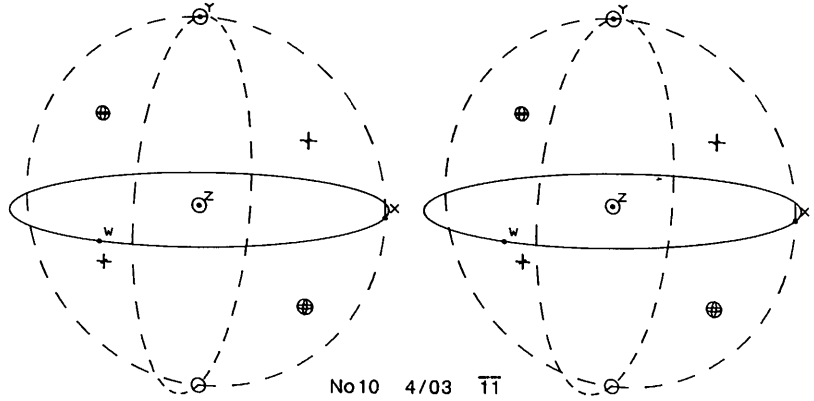


No8 4/01 mm

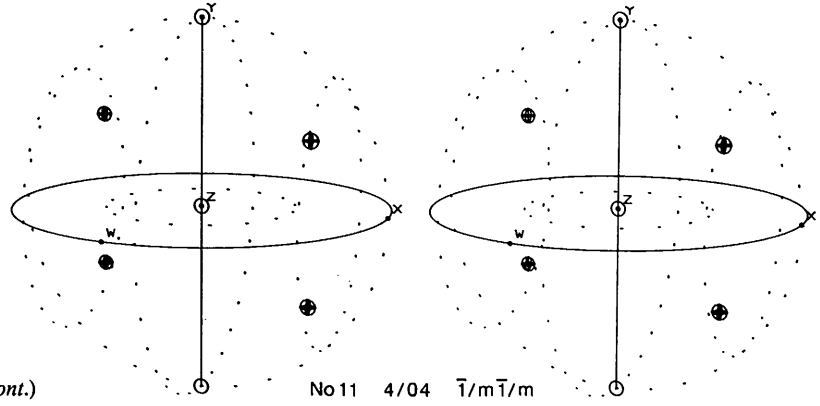
FAMILY IV MONOCLINIC SYSTEM 4 (*cont.*)



No9 4/02 $\bar{1}$m

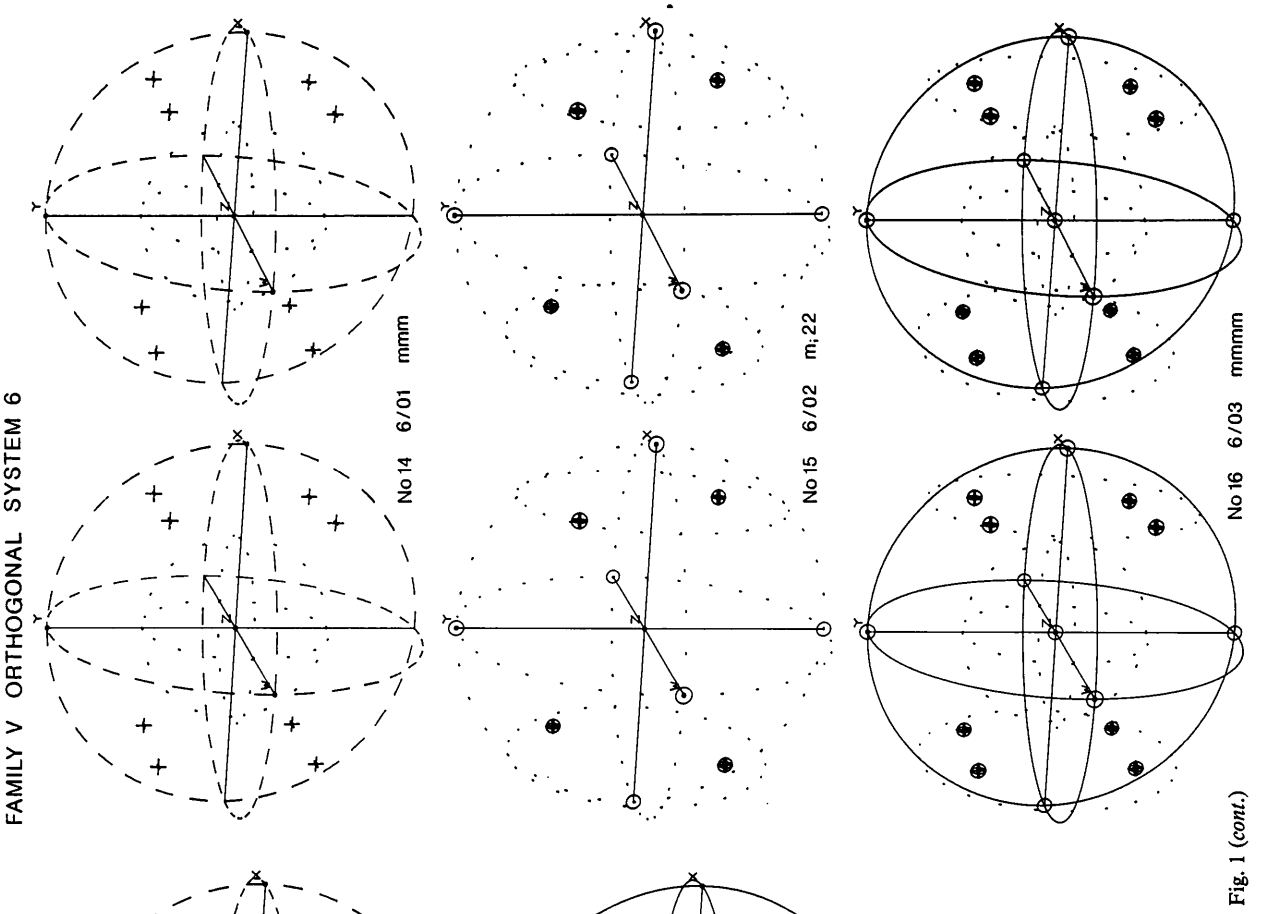


No10 4/03 $\bar{1}\bar{1}$



No11 4/04 $\bar{1}$/m$\bar{1}$/m

Fig. 1 (*cont.*)


FAMILY V ORTHOGONAL SYSTEM 6
No 14 6/01 mmm
No 15 6/02 m;22
No 16 6/03 mmmm

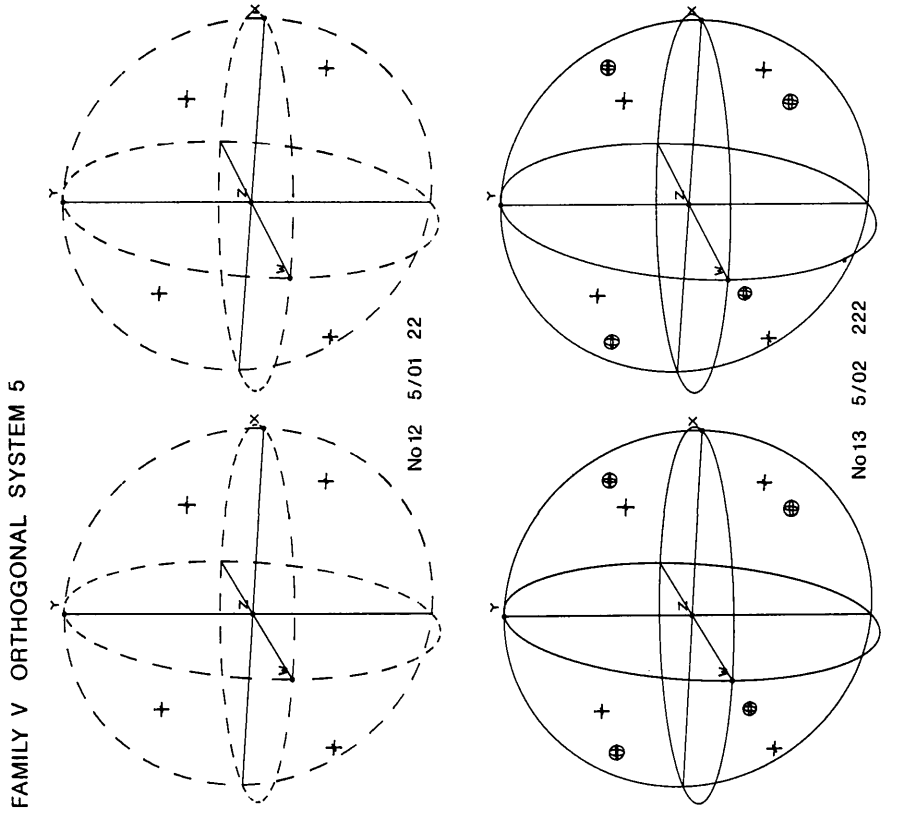

FAMILY V ORTHOGONAL SYSTEM 5
No 12 5/01 22
No 13 5/02 222

Fig. 1 (*cont.*)

Table 1. *Nomenclature for the four-dimensional crystal classes that involve symmetry elements not greater than* 2

Ordinal no.	Brown *et al.* (1978)	Symbol	Extended symbol if different	Order of group	Symmetry elements represented in Fig. 1
Family I. Hexaclinic					
System 1					
1	1/01	$\underline{1}$		1	None
2	1/03	$\tilde{\bar{1}}$		2	None
Family II. Triclinic					
System 2					
3	2/01	m		2	m on $z=0$
4	2/02	$\bar{1}$		2	$\bar{1}$ at z
5	2/03	$\bar{1}/m$		4	$\bar{1}$ at z and m on $z=0$
Family III. Diclinic					
System 3					
6	3/01	2		2	2 on wz
7	3/02	2–2		4	2 on wx and yz
Family IV. Monoclinic					
System 4					
8	4/01	mm	mm; 2	4	m on $y=0$ and $z=0$; 2 on wx
9	4/02	$\bar{1}m$	$\bar{1}m$; 2	4	$\bar{1}$ at y, m on $z=0$; 2 on yz
10	4/03	$\bar{1}\bar{1}$	$\bar{1}\bar{1}$; 2	4	$\bar{1}$ at $\pm y, z$; 2 on wx
11	4/04	$\bar{1}/m\ \bar{1}/m$	$\bar{1}/m\ \bar{1}/m$; 2–2	8	$\bar{1}$ at $\pm y, z$, m on $y=0$ and $z=0$; 2 on wx and yz
Family V. Orthogonal					
System 5					
12	5/01	22	22–2	4	2 on yz, zw and xz
13	5/02	222	222222	8	2 on wx, xy, yz, zw, wy and xz
System 6					
14	6/01	mmm	$mmm\bar{1}$; 22–2	8	m on $w=0$, $x=0$, and $y=0$; 2 on yz, xw and xy
15	6/02	$\bar{1}\bar{1}\bar{1}m$	$\bar{1}\bar{1}\bar{1}m$; 22–2	8	$\bar{1}$ at $\pm w, \pm x, \pm y$, m on $z=0$; 2 on yz, zw and xz
16	6/03	$mmmm$	$\bar{1}/m\ \bar{1}/m\ \bar{1}/m\ \bar{1}/m$; 222222	16	$\bar{1}$ at $\pm w, \pm x, \pm y$, m on $w=0$, $x=0$, $y=0$, $z=0$; 2 on wx, xy, yz, zw, wy, xz

The effects of the symmetry element operations in the 16 crystal classes illustrated are very simple.

When a mirror is represented on an axial plane this plane acts as an ordinary mirror plane in the space of the hyperstereogram.

A mirror represented on the primitive reflects a point inside the primitive to a point on a radial line and outside the primitive at an equal distance in terms of the metric of the stereographic ruler. When re-projected this becomes a point of opposite z coordinate coincident with the original point.

When a twofold rotation plane contains the z axis it is represented as a diameter of the primitive, and this diameter acts as an ordinary rotation axis in the space of the hyperstereogram.

When a rotation plane is perpendicular to the z axis it is represented as a great circle of the primitive. In order to visualize its effect, consider a central section perpendicular to this great circle and passing through the general point. This section can then be regarded as an ordinary stereogram containing a rotation axis at its point of intersection with the great circle.

An axis of $\bar{1}$ rotation–inversion located on any particular axis leads to a change of sign of all the coordinates other than the one relating to that axis. Thus $\bar{1}$ on z gives inversion of a positive point to a positive point, through the centre of the figure; $\bar{1}$ on y is equivalent to rotation around the vertical axis and change of a positive to a negative point.

A $\tilde{\bar{1}}$ point gives rise to inversion through the centre of the figure accompanied by the change of a positive to a negative point.

Application of these principles to the repetition of the crystallographic axes makes it delightfully clear how the symmetry imposes particular restrictions on the inter-axial angles in each crystal family.

A nomenclature of the crystal classes

The main difficulty in the way of a Hermann–Mauguin style nomenclature in four dimensions is that the orientation of a plane is not specifiable by the direction of a line perpendicular to it. However, mirror hyperplanes can be specified in this way. Thus, in the systems under discussion, one may look along each axis in turn (in the order w, x, y, z) and specify the presence of a rotation–inversion axis and/or a mirror in the usual way. If the fullest possible specification is required (*e.g.* to specify the choice of orientation of the axes with

respect to the symmetry) then a null symbol (–) can be written to correspond to directions in which no symmetry is present. However, since each axis is identically related to every other there is no loss of information, except that relating to orientation, if the null symbols are omitted. Thus class No. 3 (Fig. 1) is shown in the orientation ––– *m*, but *m* is a sufficient symbol.

Rotation planes have to be specified in a separate sequence. The order adopted for the axial plane is *wx*, *xy*, *yz*, *zw*, *wy*, *zx*, and a semi-colon is placed between the two series of symbols when both are present.

Again, null symbols can be inserted as required to give an unambiguous notation, including orientation. A possible shortened notation that does not include orientation may be derived as follows:

If there is only one rotation plane as in No. 6 all the null symbols may obviously be omitted.

In four dimensions two planes may intersect in a line or only in a point, and in the latter case their representations in the hyperstereogram do not intersect at all. This means that the axial planes concerned do not contain a common axis, and there are three differently oriented possibilities for No. 7, where this is true, namely 2–2–––, –2–2–– and ––––22. On the other hand, for No. 12 there are four differently oriented possibilities 22–––2, –22–2–, ––22–2 and 2––22–. If we make a convention that an orientation is chosen such that two planes are in the first four positions then No. 7 has two places occupied that are separated by a null symbol, whereas No. 12 always has two adjacent occupied places amongst these four (treated cyclicly). Thus we may symbolize No. 7 as 2–2 and No. 12 as 22 (since two two-fold planes in the latter relationship necessarily imply the third). Thus in the sequence of symbols for rotation planes it is essential to retain a null symbol when the planes involved do not intersect in a line.

Two sets of symbols for the first 16 classes are given in Table 1; 'extended symbols' are already in the shortened form discussed above. In the column headed 'symbol' the contraction has been taken a stage further by omission of those symmetry elements that are necessarily implied by others. Their meaning will be greatly clarified by comparison with the hyperstereograms in Fig. 1. Additional complications in the nomenclature arise in some higher-symmetry systems, but these will be dealt with in a subsequent publication along with the corresponding explanatory hyperstereograms.

Conclusion

The hyperstereogram is a very powerful tool in clarifying the concepts of four-dimensional crystallography.

Thanks are due to P. M. de Wolff for extremely helpful advice on improvements in the precision and clarity of presentation of the discussion.

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On the Choice of the Model Cell and the Integration Volume in the Use of the Rotation Function

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Abstract

In the general case where there is only one molecule in the asymmetric unit, and in the absence of non-crystallographic symmetry, molecular-replacement (MR) techniques can be used to solve an unknown crystal structure from a closely related known molecular model. The procedure comprises two stages in order to find (i) the orientation of the model in the crystal, and (ii) the position of the well oriented model relative to the crystallographic symmetry elements. The most widely used rotation function $R(\theta)$ [Rossmann &

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