constant for a given angular displacement from the rotation plane. This result reduces to the kind of toroidal rotation discussed previously when the projection of the rotation plane lies on the primitive, and to an ordinary rotation when it is a diameter of the primitive.

Conclusion

The properties of the hyper-stereogram that have been described provide the necessary groundwork for its use in the description of four-dimensional crystallographic symmetry, and this will be discussed in the following paper (Whittaker, 1973).

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A Representation of Hyper-Cubic Symmetry and its Projections

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The symmetry elements of the four-dimensional hyper-cube are represented in a hyper-stereogram. This is used to classify the special and general directions in holosymmetric hyper-cubic symmetry. Projections of the hyper-cube in these various directions are constructed, with the incorporation of colour perspective, and the two-colour Shubnikov symmetry of these projections is tabulated and related to the four-dimensional symmetry elements on which the projection directions lie. The general representation of other four-dimensional symmetry elements in the hyper-stereogram is discussed, and the convenience of the hyper-stereogram for facilitating the evaluation of the matrices of symmetry operations in non-standard orientations is demonstrated.

There has recently been much development in the theoretical understanding of four-dimensional crystallography and in the derivation of the four-dimensional crystal classes (*e.g.* Belov & Kuntsevich, 1971; Neubüser, Wondratschek & Bülow, 1971*a*, *b*, *c* and references therein). This work has been done in terms of the matrix representations of symmetry operations, but it is of some interest to be able to visualize the geometrical relationships of the corresponding four-dimensional symmetry elements just as we do in three dimensions, especially for the higher-symmetry crystal classes. The possibility of doing this conveniently is provided by the hyper-stereogram (Whittaker, 1973).

1. Nomenclature

The nomenclature of four-dimensional symmetry operations has hitherto been in terms of arbitrary letters (Hurley, 1951), the parameters of the characteristic equation of their matrices (Hurley, 1951), a sequence of up to four symbols representing the multiplicities of their irreducible components (Hermann, 1949), or a pair of (Cyrillic) letters indicating the general nature of the operation qualified by numerical subscripts (Kuntsevich & Belov, 1968). Since the numerical subscripts of Kuntsevich & Belov are all different they suffice as symbols in their own right. This not only simplifies the nomenclature, but also clarifies the relationship of the four-dimensional symmetry operations and elements to those in three dimensions.

In order to avoid ambiguity in this relationship it is however necessary to make two minor changes. The subscripts $\bar{n}$ of Kuntsevich & Belov are combinations of an n-fold rotation with a mirror reflexion, and are related to three-dimensional n-fold rotation–reflexion axes, not n-fold rotation–inversion axes. They have therefore been changed in this paper to $\tilde{n}$, and this nomenclature is also used for three-dimensional rotation–reflexion axes to distinguish them from $\bar{n}$-rotation–inversion axes. The other change arises because Kuntsevich & Belov retained Hermann's nomenclature of 5 and 10 for the pentatope, and a related, operation. To make clear the distinction from the non-crystallographic fivefold and tenfold rotation planes these have been replaced by V and X.

2. The hyper-stereogram of the hyper-cubic holosymmetry

The hyper-stereogram is shown, as a stereo pair, in Fig. 2. The nomenclature of the axes of Fig. 2 is shown in Fig. 1. Planes of rotation symmetry project in the hyper-stereogram as lines, and are distinguished both by cross section and colour as follows: projections of fourfold planes are shown by square-section bars in red, those of threefold planes by round rods in yellow, and those of twofold planes by flat strips in blue.

The fourfold rotation planes of the hyper-cube lie in the six axial planes defined by taking all possible combinations of the axes two at a time, and constitute three pairs of planes whose members are absolutely perpendicular, namely wx, yz; wy, zx; and xy, zw. In the hyper-stereogram the first member of each pair appears as one of the three axial great circles $WXW'X'$, $WYW'Y'$, $XYX'Y'$ of the primitive, and the second member as the diameter of the primitive perpendicular to it.

There are 36 twofold rotation planes which occur in two groups. In the first group, of 24, each contains one of the axes and a line lying in the plane of two other axes and bisecting the angle between them. These are represented by:

(i) Six great circles of the primitive bisecting the angles between the axial planes. These represent the twofold rotation planes each containing one of the axes w, x, y and a line bisecting the angle between the other two.

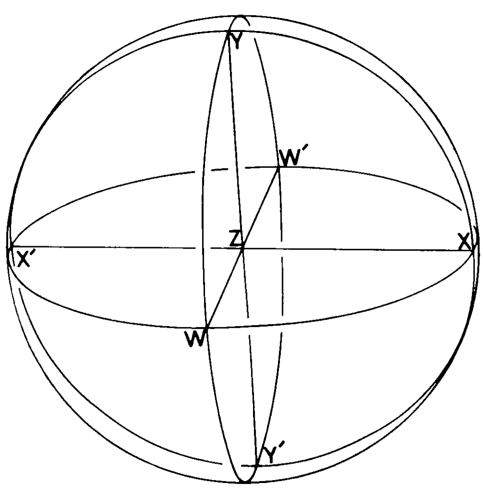

Fig. 1. Nomenclature of the axial points in Fig. 2.

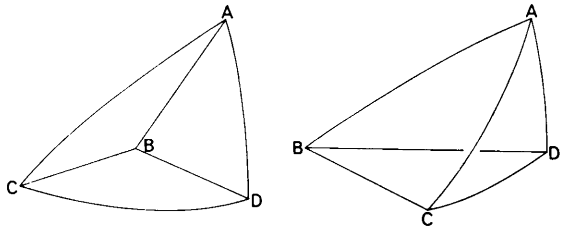

Fig. 3. Nomenclature of the representative tetrahedron outlined in white in Fig. 2: (*a*) oriented as in Fig. 2; (*b*) oriented as in Fig. 7.

(ii) Six diameters of the primitive lying in the axial planes and bisecting the angles between the axes. These represent the twofold rotation planes containing the z axis.

(iii) 12 'great circles' (in the sense in which this term is used in the ordinary stereogram) lying in the axial planes, passing through opposite ends of one axis and intersecting the perpendicular axis at a point 45° (in terms of the Wulff net) from the centre. These represent twofold rotation planes each containing one of the axes w, x, y and a line bisecting the angle between the z axis and one of the other two.

In the second group of 12, each contains a line bisecting the angle between two of the axes and a line bisecting the angle between the other two. They are represented by 'great circles' lying on the planes bisecting the angles between the axial planes of the hyper-stereogram, and passing through the ends of the diameter in (ii) above and the point 45° from the centre (in terms of the Wulff net) along the perpendicular (axial) diameter.

The 16 threefold rotation planes* each contain one of the w, x, y, z axes and a line equally inclined to the other three. Those which contain the z axis are represented by diameters of the primitive and intersect it at a point in the centre of each axial octant. The four that contain the w axis lie in the planes bisecting the angle between the WX and WY planes and pass through the point on the XY plane equidistant (in terms of the metric of the Wulff net) from Z and one end or other of XX', YY'. Similar descriptions apply, *mutatis mutandis*, to the representations of the other threefold rotation planes that contain either the x or y axis.

The mirror hyper-planes are represented in the hyper-stereogram by spherical or planar surfaces. These are not shown directly in Fig. 2 as they would obscure other parts of the model, but their locations are easily recognised because the representations of the planes of rotation symmetry form networks upon them. The 16 mirror hyper-planes may be conveniently divided into the following groups:

(i) One containing the w, x, and y axes is represented by the primitive.

(ii) The three that contain the z axis and two of the w, x and y axes are represented by the axial planes of the hyper-stereogram.

(iii) The six that contain the z axis, one of the w, x and y axes, and a line bisecting the angle between the other two, are represented by the planes bisecting the

* The combination of these threefold rotation planes with the 22 symmetry point that is also present actually leads to 62 double-rotation operations. The orientation of these could be represented by a combination of virtual $\tilde{6}$-fold rotation planes in place of the threefold planes, combined with virtual twofold rotation planes absolutely perpendicular to them. However the description of threefold planes is simpler. The situation is analogous to the conversion of a threefold rotation axis to a $\bar{3}$ rotation–inversion ($\tilde{6}$ rotation–reflexion) when combined with a centre of symmetry.

angles between the axial planes of the hyper-stereogram.

(iv) The six that contain two of the w, x, and y axes and a line bisecting the angle between the remaining one of these axes and the z axis, are represented by 'great spheres' whose geometric centres lie on the primitive.

Each of the surfaces in (i) and (ii) contains the representations of three fourfold planes (red) and six twofold planes (blue), while each of the surfaces in (iii) and (iv) contains the representations of one fourfold plane (red), four threefold planes (yellow) and four twofold planes (blue).

The representation of symmetry elements other than rotation planes and mirror hyper-planes will be discussed in § 6.

It may be noted that the axial planes of the hyper-stereogram look very like the ordinary stereogram of the symmetry elements of cubic holosymmetry, with the symmetry planes of the latter replaced by the representations of fourfold and twofold rotation planes. A more exact anaology in fact exists. All the symmetry elements on the stereogram of cubic holosymmetry (twofold, threefold and fourfold rotations and mirrors) correspond in nature and position to the symmetry elements that intersect an axial plane of the hyper-stereogram perpendicularly.

3. The representative tetrahedron

A representative tetrahedron is outlined in white in Fig. 2. This representative tetrahedron is repeated by the symmetry and occurs 192 times within the primitive. Allowing for the mirror hyper-plane represented by the primitive, a general position therefore occurs 384 times. The positions to which a general point is repeated may be deduced in detail by application of the constructions for reflexions in hyper-planes and rotations about planes discussed in the previous paper (Whittaker, 1973).

The representative tetrahedron is redrawn in Fig. 3(a) and its vertices lettered for reference. The position of a point within or on it may be specified as $(h_1h_2h_3h_4)$, where the values of h may be construed (if integral) as the indices of a crystallographic hyper-plane, or more generally a vector in $R4$. $\{h_1h_2h_3h_4\}$ then represents a crystallographic form or the set of symmetry related vectors.

Each face of the tetrahedron lies on the representation of a mirror hyper-plane. If the point $(h_1h_2h_3h_4)$ lies on a face its multiplicity is reduced to 192 and the vector takes one of the following forms:

on ABC: $\{h_1h_2h_2h_4\}$ with the smallest $|h|$ repeated;
on ABD: $\{h_1h_1h_3h_4\}$ with the intermediate $|h|$ repeated;
on ACD: $\{h_1h_2h_3h_1\}$ with the largest $|h|$ repeated;
on BCD: $\{h_1h_20h_4\}$.

If the point lies on one of the edges of the tetrahedron the multiplicity is further by reduced the order of the symmetry element on that edge, and takes the following forms:

AB	64	$\{h_1h_1h_1h_4\}$
AC	96	$\{h_1h_2h_2h_1\}$
AD	64	$\{h_1h_1h_3h_1\}$
BC	48	$\{h_100h_4\}$
BD	96	$\{h_1h_10h_4\}$ with $\|h_1\| < \|h_4\|$
CD	96	$\{h_1h_20h_1\}$ with $\|h_1\| > \|h_2\|$.

If the point lies at a vertex the following cases arise:

A	16	$\{1\ 1\ 1\ 1\}$
B	8	$\{0\ 0\ 0\ 1\}$
C	24	$\{1\ 0\ 0\ 1\}$
D	32	$\{1\ 1\ 0\ 1\}$.

4. Projections with colour perspective

All the information about a four-dimensional geometric figure can be represented in three dimensions provided that some continuously variable parameter, proportional to the fourth coordinate (perpendicular to the other three) can be associated with each point. An obvious possibility for the required parameter is a continuous colour change which is an extension of the use by Mackay & Pawley (1963) of p colours to represent points at p levels. The principle is conveniently demonstrated by applying it to the representation of a cube in two dimensions. Fig. 4 shows seven projections of a cube; the projection directions map at the vertices, on the edges, and within, the representative triangle (shown by bold lines) on the inset stereogram of the symmetry elements of the cube. The projections are arranged relative to one another in accordance with the position on the representative triangle of the mapping of their respective projection directions.

A continuously variable colour parameter, ranging from orange–red, through yellow and green, to blue, is assigned to each point of a projection corresponding to the distance of the corresponding point of the cube from the observer in the third dimension perpendicular to the plane of the projection. This spectral sequence was chosen to give some correspondence to the usual 'blueing with distance' that is the basis of colour perspective in landscape painting. In cases when two edges of the cube map on to the same line in projection, and the appropriate colour coordinates are equally and oppositely displaced from the mid-green, the line is shown in grey.

Fig. 5 and Fig. 6 show similarly coloured three-dimensional models of the four-dimensional hyper-cube. Fig. 5 is the projection down a [1111] direction (vertex A of the representative tetrahedron of Fig. 3), and Fig. 6 is the projection down a general direction that maps in the interior of the representative tetrahedron.

There are in all 15 different kinds of projection of the hyper-cube, corresponding to the positions in the representative tetrahedron at which the projection direction may map, as listed in § 3. The models of all these

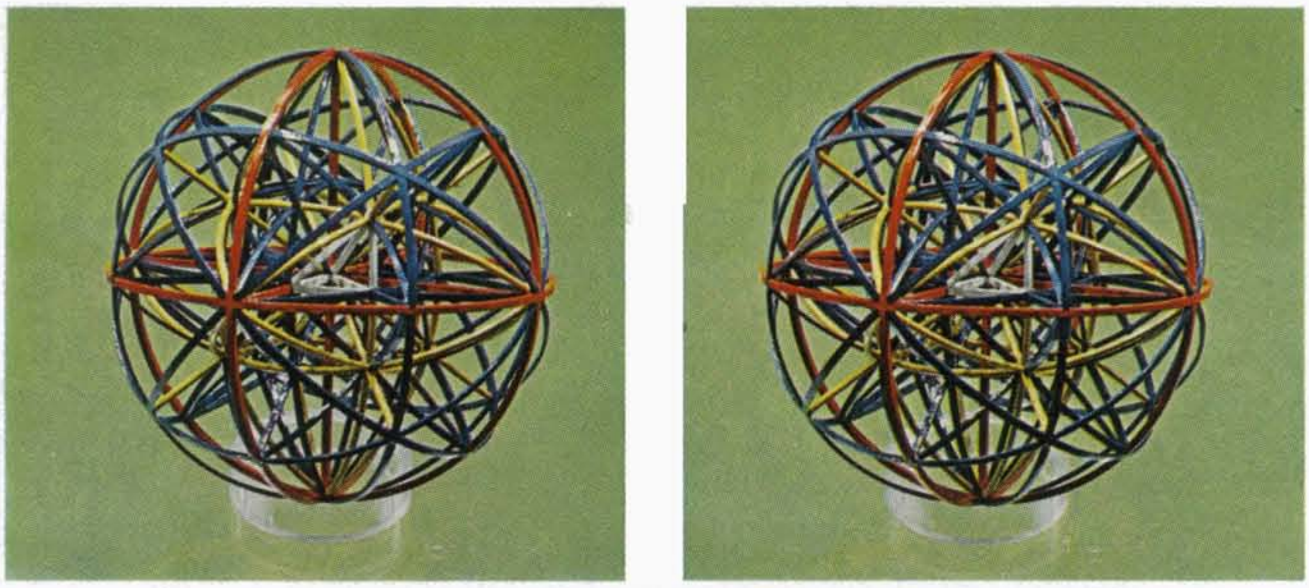

Fig. 2. The hyper-stereogram of the hyper-cubic holosymmetry. Square section (red) represents fourfold rotation planes; round section (yellow) represents threefold rotation planes; flat section (blue) represents twofold rotation planes. A representative tetrahedron is outlined in white.

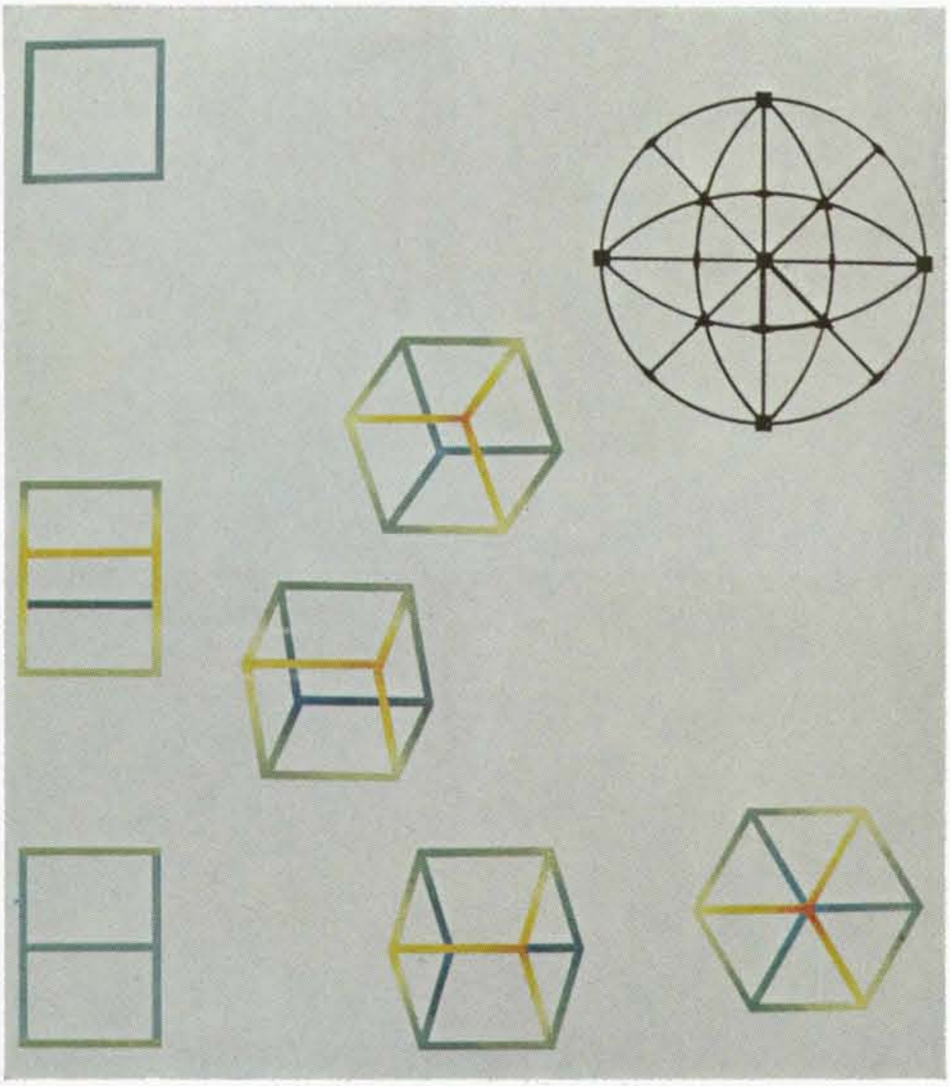

Fig. 4. Projections of the cube, with a colour parameter (red, through yellow and green, to blue) to represent increasing distance perpendicular to the projection plane. The seven projection directions are indicated by corresponding points on the heavily outlined representative triangle in the stereogram of the cubic holosymmetry.

projections are shown in Fig. 7 arranged relative to one another in accordance with the position in the representative tetrahedron [oriented as in Fig. 3(*b*)] of the mappings of their respective projection directions.

5. Symmetry of the projections

Although the diagrams of Fig. 4 and the models of Fig. 7 are multicoloured, their symmetry can be considered in terms of the Shubnikov two-colour point groups: change of colour is understood as an inversion between two colour values equally separated to the orange and blue sides of mid-green.

It is evident from Tables 1 and 2 that there is a close relationship between the colour symmetry of a projection and the symmetry elements on which the projection direction lies, but this relationship is not entirely straightforward. The matter can be elucidated further for individual crystallographic symmetry operations by repetitive multiplication of an arbitrary vector by the matrix of the symmetry operation. If the set of values of any component (or any subset of it) remains unchanged in magnitude, this indicates a relevant projection direction. For projections from $R3$ to $R2$ this reveals the relationships shown in Table 3 from which it can be seen that projection directions perpendicular to symmetry elements may also result in symmetry in the projection. The reason for this is that symmetry in the projection can arise not only when the direction of projection is truly invariant under the symmetry operation but also when it is merely confined to a line or a plane.

Table 1. *Colour point groups of the projections of a cube in Fig. 4 compared with the symmetry elements on which the projection direction lies*

A is taken as the position on the stereogram of the 3 axis and B of the 4 axis.

Three-dimensional symmetry elements coincident with projection direction		Two-dimensional colour point group of projection
At A	$\bar{3}$ axis ($\tilde{6}$) axis); three m planes	$6'mm'$
B	4 axis; four m planes	$4mm$ (grey)
C	2 axis; two m planes	$2mm$ (grey)
On AB	m plane	mm'
BC	m plane	mm'
CA	m plane	mm'
In ABC	$\bar{1}$ centre (also present in all)	$2'$

Table 3. *Two-colour two-dimensional symmetry in projections (with colour perspective) of three-dimensional symmetry elements*

Symmetry element along $\mathbf{z}$	Projection parallel to $\mathbf{z}$	Projection perpendicular to $\mathbf{z}$
$m\,(\perp\mathbf{z})$	grey	$m\,(\perp\mathbf{z})$
2	2	$m\,(\parallel\mathbf{z})$
3	3	—
4	4	$m\,(\parallel\mathbf{z})$
6	6	$m\,(\parallel\mathbf{z})$
$\tilde{2}\,(\bar{1})$	$2'$	$2'$
$\tilde{3}\,(\bar{6})$	3 grey	$m\,(\perp\mathbf{z})$
$\tilde{4}\,(\bar{4})$	$4'$	$m'(\parallel\mathbf{z})$
$\tilde{6}\,(\bar{3})$	$6'$	$2'$

Table 4 gives the corresponding relationships for projection from $R4$ to $R3$ of all the 23 crystallographic symmetry operations other than the identity. Here, extended conditions become even more important because for many of the symmetry operations the only invariant symmetry element is a point, but there may nevertheless be a number of projection directions in which some symmetry is retained.

The results in Tables 1 and 2 can all be explained in terms of Tables 3 and 4 with three exceptions. The first of these is the presence of 4′ axes in projection A of Table 2, which corresponds to the model of Fig. 5. These 4′ axes are due to the existence of coincident symmetry elements along each of the eight diagonals of the hyper-cube. These are the invariant lines of $\tilde{4}$ symmetry operations. No symmetry axes were repre-

Table 2. *Colour point groups of the projections of a hyper-cube in Fig. 7 compared with the four-dimensional symmetry elements on which the projection direction lies*

4 D symmetry elements coincident with projection directions		3D colour point group of model
At A	four 3 planes; three 2 planes; six m hyperplanes.	$4'3\,2'$
B	three 4 planes; four 3 planes; six 2 planes; nine m hyperplanes.	$m3m$ grey ($4/m\,\tilde{6}\,2/m$)
C	one 4 plane; four 2 planes; five m hyperplanes.	$4/m\,m\,m$ (grey)
D	one 3 plane; three 2 planes; four m hyperplanes.	$6'/m\,m'm$
On AB	one 3 plane; three m hyperplanes.	$\bar{3}'m$ ($\tilde{6}'m$)
AC	one 2 plane; two m hyperplanes.	$2/m'm\,m$
AD	one 3 plane; three m hyperplanes.	$\bar{3}'m$ ($\tilde{6}'m$)
BC	one 4 plane; four m hyperplanes.	$4/m'm\,m$
BD	one 2 plane; two m hyperplanes.	$2/m'm\,m$
CD	one 2 plane; two m hyperplanes.	$2/m'm\,m$
On ABC	one m hyperplane.	$2'/m$
DAB	one m hyperplane.	$2'/m$
CDA	one m hyperplane.	$2'/m$
BCD	one m hyperplane.	$2'/m$
In $ABCD$	the 22 double rotation (also present additionally on all the others)	$\bar{1}'$ ($\tilde{2}'$)

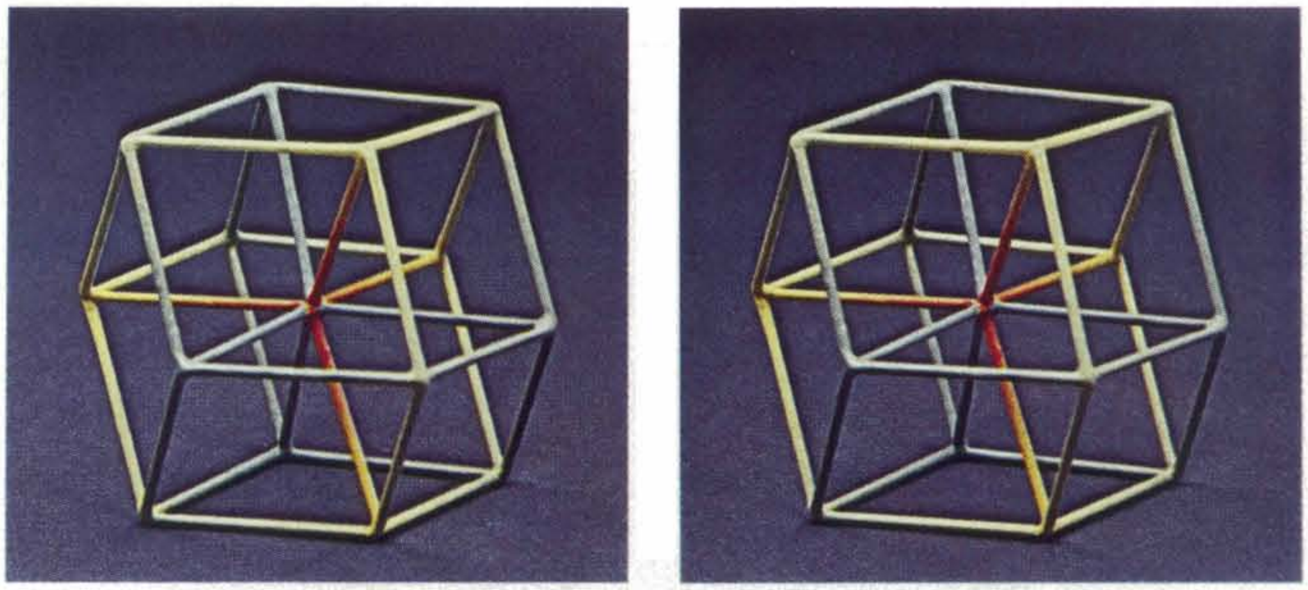

Fig. 5. Projection of the hyper-cube down a direction making equal angles with the four axes. The colour parameter (red, through yellow and green, to blue) represents increasing distance perpendicular to all three dimensions of space.

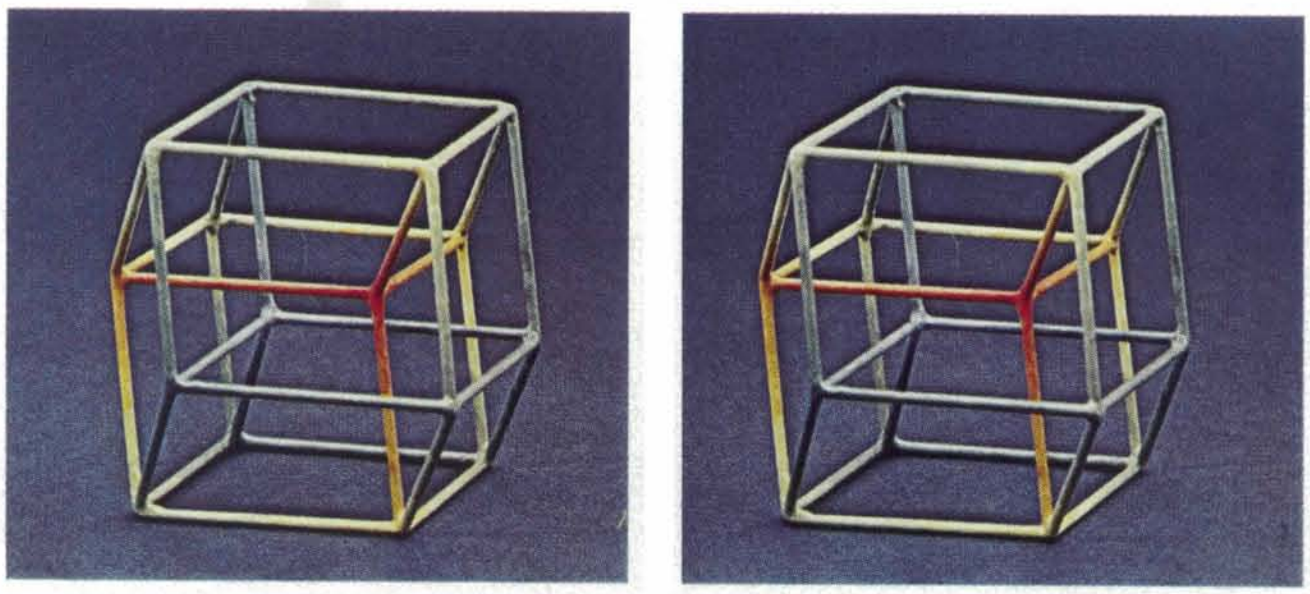

Fig. 6. Projection of the hyper-cube in a general direction (with colour perspective).

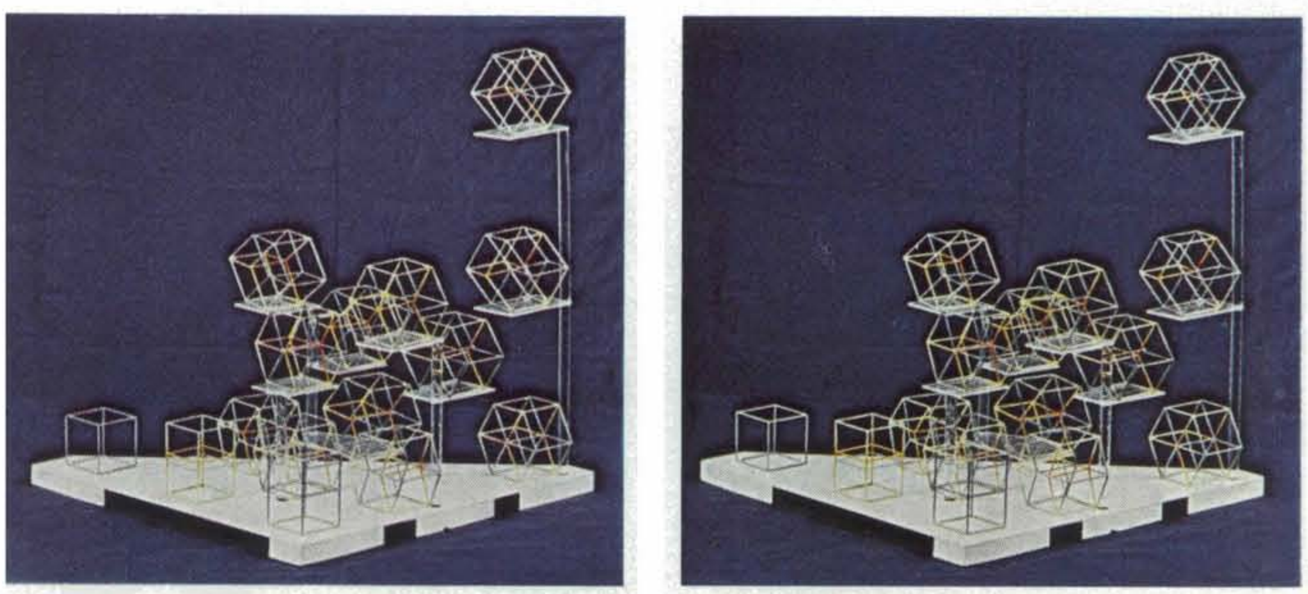

Fig. 7. Fifteen projections of the hyper-cube (with colour perspective). The projection directions are indicated by corresponding points on the white representative tetrahedron in the hyper-stereogram of Fig. 2.

sented in the hyper-stereogram of Fig. 2 but we can now see that this should have been done at the intersections in each octant of the four representations of threefold planes. For reasons that will appear in the next section, a suitable representation would be an outline tetrahedron surrounding each of these eight points, with the representations of the threefold planes emerging along its threefold axes. This would correctly represent the nature and orientation of the $\tilde{4}$ symmetry axes, and would further enhance the analogy of Fig. 2 to the classical stereogram of cubic holosymmetry.

The second exception is the presence of $\bar{3}$ axes ($\tilde{6}$ axes) in the grey cube of projection *B*. This is due to the presence of four coincident symmetry axes of type $\tilde{6}$ along [0001] (and related axes). These should similarly be represented by an outline cube surrounding the relevant points in the hyper-stereogram. The third exception is the presence of a $6'$ axis in the projection at *D*. This arises because the combination of the 3 plane along *AD*, the perpendicular *m* hyper-plane in *BCD*, and the 22 symmetry point give rise to a $\tilde{6}$ axis at *D*.

6. The representation of symmetry axes

It has been possible to deduce directly from the preceding paper (Whittaker, 1973) how to represent not only the symmetry elements of mirror hyper-planes and *n*-fold rotation planes, but also the effect of their operation. However, these symmetry elements correspond to only nine of the 23 crystallographic symmetry operations (other than the identity) that exist in *R*4. There are a further four symmetry operations that have an invariant line, and whose symmetry element is therefore an axis. These are $\tilde{2}$, $\tilde{4}$, $\tilde{3}$ and $\tilde{6}$ axes. Each may be regarded as a product of two operations $\mathsf{M}_{134}.\mathsf{R}_{12}$, where R is a rotational symmetry operation (of appropriate order), M is a reflexion operation, and the subscripts denote four orthogonal directions, of which 1 specifies the invariant axis of the whole operation, 1 and 2 together define the invariant plane of R, and 1, 3 and 4 the hyper-plane of M.

It is therefore evident that such a symmetry element can be represented by a point in the hyper-stereogram and its operation can be defined geometrically by a combination of a rotation about the line representing the rotation plane of R and a reflexion in the surface representing the mirror hyper-plane of M, as defined in the preceding paper (Whittaker, 1973). In a simple case where the axes 1, 2, 3, 4 coincide with some permutation of *w*, *x*, *y*, *z* there would be little difficulty in identifying such operations in the hyper-stereogram, but in the case of the $\tilde{4}$ axes discussed in the previous section the directions of the axes 2, 3, 4 are by no means obvious. However reference to the hyper-stereogram greatly simplifies the problem.

Table 4. *Two-colour three-dimensional symmetry in projections (with colour perspective) of four-dimensional symmetry elements*

	Projection direction						
Symmetry element	$\parallel$**z**	$\parallel$**y**	In *yz*	In *wx*	$\perp$**z**	$\perp$**y**	General
m ($\perp$**z**)	grey	*	–	*	m($\perp$**z**)	–	–
2 (*yz*)	*	*	2 (in *yz*)	m' (*yz*)	–	–	–
3 (*yz*)	*	*	3 (in *yz*)	–	–	–	–
4 (*yz*)	*	*	4 (in *yz*)	m' (*yz*)	–	–	–
6 (*yz*)	*	*	6 (in *yz*)	m' (*yz*)	–	–	–
$\tilde{2}$ (**z** with reflexion $\perp$**y**)	$\tilde{2}$ (**y**)	*	–	*	$2'$ (**z**)	–	–
$\tilde{3}$ (**z** with reflexion $\perp$**y**)	$\tilde{3}$ (**y**)	3 grey(**z**)	3 (in *yz*)	*	–	m ($\perp$**y**)	–
$\tilde{4}$ (**z** with reflexion $\perp$**y**)	$\tilde{4}$ (**y**)	$4'$ (**z**)	2 (in *yz*)	m' (*yz*)	–	–	–
$\tilde{6}$ (**z** with reflexion $\perp$**y**)	$\tilde{6}$ (**y**)	$6'$ (**z**)	3 (in *yz*)	*	$2'$ (**z**)	–	–
22 (*yz–wx*)	*	*	*	*	*	*	$\tilde{2}'$
32 (*yz–wx*)	*	*	$\tilde{3}'$ (in *yz*)	2 (in *wx*)	–	–	–
42 (*yz–wx*)	*	*	$\tilde{4}'$ (in *yz*)	m' (*yz*)	–	–	–
62 (*yz–wx*)	*	*	$\tilde{6}'$ (in *yz*)	*	*	*	$\tilde{2}'$
33 (*yz–wx*)	–	–	–	–	–	–	–
43 (*yz–wx*)	*	*	4 (in *yz*)	$\tilde{3}'$ (in *wx*)	–	–	–
63 (*yz–wx*)	–	–	2 (in *yz*)	m' (*yz*)	–	–	–
44 (*yz–wx*)	*	*	*	*	*	*	$\tilde{2}'$
64 (*yz–wx*)	*	*	$\tilde{3}'$ (in *yz*)	$\tilde{4}'$ (in *wx*)	–	–	–
66 (*yz–wx*)	*	*	*	*	*	*	$\tilde{2}'$
444	*	*	*	*	*	*	$\tilde{2}'$
3344	–	–	–	–	–	–	–
V	–	–	–	–	–	–	–
X	*	*	*	*	*	*	$\tilde{2}'$

Notes: (1) When a particular projection direction does not lead to any different symmetry from a more general projection direction this is indicated by an asterisk; the symmetry arising is given by the first following positive entry.

(2) The direction of an axis specified in columns 4 or 5 as 'in *yz*' or 'in *wx*' is the direction in the plane *yz* or *wx* perpendicular to the projection direction.

The symmetry operation involved arises (just like the $\bar{4}$ axis in the cubic class $\bar{4}32$) by the combination of a threefold rotation plane with a mirror hyper-plane.

Consider the threefold rotation plane along AB (Figs. 2 and 3) and the mirror hyper-plane through A that reflects Y to Z. The former clearly transforms $(1000) \rightarrow (0100) \rightarrow (0010)$ and leaves (0001) unchanged, so that the matrix of the $\tilde{4}$ operation arising from their combination is evidently given by

$$\begin{pmatrix}1000\\0100\\0001\\0010\end{pmatrix}\begin{pmatrix}0010\\1000\\0100\\0001\end{pmatrix}=\begin{pmatrix}0010\\1000\\0001\\0100\end{pmatrix}.$$

It may readily be verified that this matrix is also the product of those corresponding to a virtual fourfold rotation plane along AC and a mirror hyper-plane containing the two other blue lines intersecting at A (Fig. 2). The effects of such operations can easily be seen from the hyper-stereogram to be: a fourfold plane along AC transforms $(0\bar{1}00) \rightarrow (100\bar{1}) \rightarrow (01\bar{1}0) \rightarrow (\bar{1}001)$; the required hyper-plane passes through (1010), (1100) and (0110) and so transforms them to themselves. These observations on the hyper-stereogram lead directly to the matrices

$$\tfrac{1}{2}\begin{pmatrix}1\bar{1}11\\111\bar{1}\\\bar{1}111\\11\bar{1}1\end{pmatrix} \quad\text{and}\quad \tfrac{1}{2}\begin{pmatrix}111\bar{1}\\11\bar{1}1\\1\bar{1}11\\\bar{1}111\end{pmatrix} \text{ respectively, and}$$

their product is the same as above.

Thus each of the three $\tilde{4}$ symmetry elements at A corresponds to a virtual fourfold rotation about one of the twofold rotation planes through A combined with a reflexion in the hyper-plane defined by the other two. The effect of this on a point in the hyper-stereogram is most simply described as a repetition at the vertices of a tetrahedron surrounding A, and tending to a regular tetrahedron centred on A as the points approach A.

The derivation of the four coincident $\tilde{6}$ axes along $[0001]$ (and related axes) can be derived similarly. As a result of combining the threefold rotation plane along AB (whose matrix was derived above) with the three axial mirror hyper-planes that intersect it at B one obtains:

$$\begin{pmatrix}\bar{1}000\\0100\\0010\\0001\end{pmatrix}\begin{pmatrix}1000\\0\bar{1}00\\0010\\0001\end{pmatrix}\begin{pmatrix}1000\\0100\\00\bar{1}0\\0001\end{pmatrix}\begin{pmatrix}0010\\1000\\0100\\0001\end{pmatrix}=\begin{pmatrix}00\bar{1}0\\\bar{1}000\\0\bar{1}00\\0001\end{pmatrix}$$

which is in turn equivalent to a combination of a sixfold rotation about AB and a mirror hyper-plane perpendicular to it as shown by the product

$$\tfrac{1}{9}\begin{pmatrix}1\bar{1}\bar{1}0\\\bar{2}1\bar{2}0\\\bar{2}\bar{2}10\\0001\end{pmatrix}\begin{pmatrix}22\bar{1}0\\\bar{1}220\\2\bar{1}20\\0001\end{pmatrix}=\begin{pmatrix}00\bar{1}0\\\bar{1}000\\0\bar{1}00\\0001\end{pmatrix}.$$

7. The representation of point symmetry elements

The remaining ten kinds of four-dimensional symmetry operation do not leave any vector invariant, and their symmetry element is therefore only a point at the origin. However, this statement would also be true of $\tilde{n}$-axes of symmetry in three-dimensional space, but except for $\tilde{n}=\tilde{2}$ these nevertheless have a directional character and it is necessary to specify the direction of the axis of their rotational component. A similar need arises in four dimensions for the representation of the planes of component rotations.

This need does not arise for the double rotation 22 whose components are two absolutely perpendicular twofold rotation planes. Its effect is independent of the orientation of these planes and is simply to change the sign of all coordinates. Since a point at the centre of the hyper-sphere does not lie on its boundary it cannot strictly be represented on the hyper-stereogram. However just as $\tilde{2}$ is conventionally represented by an open circle at the centre of a stereogram, so the point in question could appropriately be represented by a small empty sphere at the centre of the hyper-stereogram.

In all the other nine types of double rotation about a pair of absolutely perpendicular planes it is necessary to specify at least one of these planes. In a model hyper-stereogram containing them, they would obviously be represented in a similar way to true rotation planes but with some distinctive marking such as black bands. The triple rotation 444 similarly requires the specification of at least one of the two component virtual fourfold planes that are absolutely perpendicular to one another and of the third virtual fourfold plane perpendicular to both. In the hyper-stereogram the simplest example would be a great circle of the primitive, a diameter of the primitive perpendicular to this, and another great circle of the primitive through the ends of this diameter.* There are twelve differently orientated such symmetry elements in the symmetry of the hyper-cube arising from the actual fourfold planes that are present. The quadruple rotation 3344 analogously requires the specification of at least one of a pair of absolutely perpendicular threefold planes and at least one of a pair of absolutely perpendicular fourfold planes perpendicular to them.

The pentatope operation (V) again has only a point symmetry element, but its orientation in the hyper-stereogram requires to be expressed in some way. Moreover it does possess a set of five vectors which is invariant *as a set* and these serve to define its orienta-

* This is sufficient to specify the orientation provided that a suitable convention of rotation sense is adopted. The three planes outline three edges of the positive octant of the hyper-stereogram that form an open figure. If on proceeding from one end of this figure to the other the sense of rotation in the hyper-stereogram always remains the same then there is a 1:1 correspondence between the symmetry operation and the set of three planes.

tion. It is therefore most conveniently represented in the hyper-stereogram by the projections of a set of five points equidistant from one another on the hyper-sphere at $2\tan^{-1}(\sqrt{5}/\sqrt{3})$ apart. The simplest orientation which gives rise to the standard form (Mackay & Pawley, 1963),

$$\frac{1}{4}\begin{pmatrix} 1 & 1 & 3 & \sqrt{5} \\ 1 & -3 & -1 & \sqrt{5} \\ -3 & 1 & -1 & \sqrt{5} \\ -\sqrt{5} & -\sqrt{5} & \sqrt{5} & -1 \end{pmatrix}$$

for the matrix, is a point at the centre of the hyper-stereogram together with four points tetrahedrally arranged around it in the centres of the positive wxy octants at $r=\sqrt{5}/\sqrt{3}$. The effect of the V operation in the hyper-stereogram is most simply envisaged as a combination of a $\tilde{4}$ rotation axis and a reflexion in a hyper-plane making $\tan^{-1}(\sqrt{5}/\sqrt{3})$ with this axis. In the above case the $\tilde{4}$ rotation axis would be the z axis, with its rotation component about the xz plane, and the hyper-plane would be equally inclined to the w, x and y axes.

The X operation can similarly be represented by the same five points together with their opposites.

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Neutron-Diffraction Study of $Tb(OH)_3$ – A Case of Severe Extinction*

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Neutron-diffraction experiments on a single crystal of $Tb(OH)_3$ have indicated severe extinction effects. For some Bragg reflections the observed neutron cross section is attenuated by a factor of ten owing to extinction. A least-squares refinement (including extinction) of the structure factors deduced from integrated intensities measured at room temperature gives structural parameters in good agreement with a previous determination, and new information about the position and thermal vibrations of the hydrogen atom. The final residual of 0·036 indicates that extinction is well accounted for by the Zachariasen formulae, and the value of g, the extinction parameter, is $(6\pm1)\times10^4$. The polarized-neutron technique has been used to measure the ratio between the magnetic and nuclear structure factors at 2·6°K, at which temperature $Tb(OH)_3$ is ferromagnetic (9 μ_B/Tb atom). The effect of extinction is particularly dramatic in this experiment, but again the results may be explained with the simple Zachariasen correction and the same extinction parameter as used for the unpolarized data. The corrected magnetic scattering amplitudes deduced from the polarized-neutron experiment allow the magnetic form factor of the terbium atom to be found, and compared to that measured in terbium metal; this aspect of the investigation is discussed in a separate article.

Introduction

The problem of extinction in experiments concerned with measuring Bragg intensities in both X-ray and neutron diffraction has received much attention over the last few years. Recognized in the very early days of crystallography by Darwin (see James, 1958) extinction results in the stronger Bragg intensities appearing weaker than predicted by the kinematical theory. Experiments aimed at determining crystal structures are somewhat independent of this problem, since the stronger reflections are often disregarded in the refinements, and the correlation between the extinction and the final positional parameters is usually small. The most thorough treatment of extinction has been formulated by Zachariasen (1967, 1968*a*, 1968*b*). Despite doubts about the mathematical treatment (Werner, 1969), and the physical significance of the final parameters (Lawrence, 1972; Killean, Lawrence & Sharma, 1972), the Zachariasen theory has found wide acceptance among experimentalists, and is now routinely included in least-squares refinements of the structural parameters. Second-order corrections in the form of

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