trigonal and hexagonal layer and rod groups

N	3-D group	layer group	rod group
143	*P*3	*p*3	**p**3
144	$P3_1$		$\mathbf{p}3_1$
145	$P3_2$		$\mathbf{p}3_2$
147	$P\bar{3}$	$p\bar{3}$	$\mathbf{p}\bar{3}$
149	*P*312	*p*312	[**p**312 ≡ **p**321]
150	*P*321	*p*321	**p**321
152	$P3_121$		$\mathbf{p}3_121$
154	$P3_212$		$\mathbf{p}3_221$
156	*P*3*m*1	*p*3*m*1	**p**3*m*1
157	*P*31*m*	*p*31*m*	[**p**31*m* ≡ **p**3*m*1]
158	*P*3*c*1		**p**3*c*1
162	$P\bar{3}1m$	$p\bar{3}1m$	[$\mathbf{p}\bar{3}1m \equiv \mathbf{p}\bar{3}m1$]
164	$P\bar{3}m1$	$p\bar{3}m1$	$\mathbf{p}\bar{3}m1$
165	$P\bar{3}c1$		$\mathbf{p}\bar{3}c1$
168	*P*6	*p*6	**p**6
169	$P6_1$		$\mathbf{p}6_1$
170	$P6_5$		$\mathbf{p}6_5$
171	$P6_2$		$\mathbf{p}6_2$
172	$P6_4$		$\mathbf{p}6_4$
173	$P6_3$		$\mathbf{p}6_3$
174	$P\bar{6}$	$p\bar{6}$	$\mathbf{p}\bar{6}$
175	*P*6/*m*	*p*6/*m*	**p**6/*m*
176	$P6_3/m$		$\mathbf{p}6_3/m$
177	*P*622	*p*622	**p**622
178	$P6_122$		$\mathbf{p}6_122$
179	$P6_522$		$\mathbf{p}6_522$
180	$P6_222$		$\mathbf{p}6_222$
181	$P6_422$		$\mathbf{p}6_422$
182	$P6_322$		$\mathbf{p}6_322$
183	*P*6*mm*	*p*6*mm*	**p**6*mm*
184	*P*6*cc*		**p**6*cc*
185	$P6_3cm$		$\mathbf{p}6_3cm$
187	$P\bar{6}m2$	$p\bar{6}m2$	$\mathbf{p}\bar{6}m2$
188	$P\bar{6}c2$		$\mathbf{p}\bar{6}c2$
189	$P\bar{6}2m$	$p\bar{6}2m$	[$\mathbf{p}\bar{6}2m \equiv \mathbf{p}\bar{6}m2$]
191	*P*6/*mmm*	*p*6/*mmm*	**p**6/*mmm*
192	*P*6/*mcc*		**p**6/*mcc*
194	$P6_3/mmc$		$\mathbf{p}6_3/mmc$

APPENDIX 2

A GLIMPSE INTO HIGHER DIMENSIONS

A2.1 Introduction: polytopes

There are many reasons for considering structures in higher dimensions—some of them practical, some of them aesthetic. Here we can only give a few teasing hints of the richness of the geometry of higher dimensions, but it is hoped they will remove some of the irrational fear of the subject and perhaps kindle a desire to delve more deeply into the subject. Our main purposes are to introduce terms that are gaining increasing currency in crystallography and to give some insight into how higher dimensional problems are handled.

We start by generalizing a three-dimensional Cartesian axis system to n dimensions so that there are n orthogonal axes $\mathbf{a}_1, \mathbf{a}_2, \ldots \mathbf{a}_n$. The n coordinates of a point in this space are $x_1, x_2, \ldots x_n$. The Pythagoras theorem gives the distance between two points $x_{11}, x_{21}, \ldots x_{n1}$ and $x_{12}, x_{22}, \ldots x_{n2}$ as

$$d^2 = (x_{11} - x_{12})^2 + (x_{21} - x_{22})^2 + \ldots + (x_{n1} - x_{n2})^2 \qquad \text{(A2.1)}$$

The generalization of a polygon (in two dimensions) and a polyhedron (in three dimensions) to n dimensions is a *polytope*. A *hypercube* or *measure polytope* of edge b with center at the origin has 2^n vertices at $(\pm b/2, \pm b/2, \ldots, \pm b/2)$ and has content ("volume") b^n. It is an example of a *regular* polytope. It is amusing that for a four-dimensional cube (known as a *tesseract*) the distance from the center to a vertex [which is $\sqrt{(b^2/4 + b^2/4 + b^2/4 + b^2/4)}$] is equal to the edge length (b).

Another regular polytope is the *cross polytope*. For edge length b this has $2n$ vertices at $\pm(b/\sqrt{2}, 0, \ldots 0)$κ. The three-dimensional version is the regular octahedron. The volume is $V = b^n 2^{n/2}/n!$.

A third polytope of importance is the *simplex* which has $n + 1$ vertices each of which is joined to all the others by edges, so that there are $n(n + 1)/2$ edges. A two-dimensional simplex is a triangle and a three-dimensional simplex is a tetrahedron. A regular simplex has all edges equal, say b, and volume $V = b^n\sqrt{(n + 1)}/[n!2^{n/2}]$. The angle subtended by an edge at the center is $\cos^{-1}(-1/n)$ and the vertex to center distance is $b\sqrt{[n/(2n + 2)]}$. The order of the symmetry group of a regular simplex is $(n + 1)!$.

These are the only regular polytopes for $n \geq 5$, but four-dimensional space has some beautiful surprises (recall that in three dimensions we have two more regular polyhedra, the icosahedron and dodecahedron) that are mentioned below.

Points on the surface of a *hypersphere* (or just *sphere*) in n dimensions with center at the origin (0,0,...,0) and with radius r are given by:

$$r^2 = x_1^2 + x_2^2 + \ldots + x_n^2 \qquad \text{(A2.2)}$$

The volume is given by (the second form avoids non-integral factorials for odd n):

$$V = r^n \pi^{n/2}/(n/2)! = (2r)^n \pi^{(n-1)/2}[(n-1)/2]!/n! \qquad \text{(A2.3)}$$

An often useful formula is for the volume of a general simplex with vertices (in Cartesian coordinates) $(x_{01},x_{02},\ldots x_{0n})$, $(x_{11},x_{12},\ldots x_{1n})$, ..., $(x_{n1},x_{n2},\ldots x_{nn})$ [compare Eq. 4.25]:

$$V = \frac{1}{n!}\begin{vmatrix} 1 & x_{01} & \ldots & x_{0n} \\ 1 & x_{11} & \ldots & x_{1n} \\ \ldots & \ldots & & \\ 1 & x_{n1} & \cdots & x_{nn} \end{vmatrix} \qquad \text{(A2.4)}$$

The sign of V depends on the order of numbering of the vertices.

A2.2 Four-dimensional polytopes and honeycombs

It is convenient to rewrite the Schläfli symbols we have been using on one line. Thus the symbol for a cube 4^3 becomes {4,3} and an octahedron 3^4 becomes {3,4}. The symbol for a 4-dimensional hypercube becomes {4,3,3}. This is interpreted as a polytope whose hyperfaces (*cells*) are {4,3} (i.e. cubes) and three of these meet at an edge.

Two-dimensional tessellations can be considered as degenerate cases of three-dimensional polyhedra. For example {3,3}, {3,4} and {3,5} are the tetrahedron, octahedron and icosahedron respectively whereas {3,6} is a covering of the plane by (an infinite number of) triangles. Likewise {4,3} is a cube but {4,4} is a covering of the plane by squares. The other regular tessellation of the plane is {6,3}. In the same way a three-dimensional space filling by cubes (with four meeting at every edge) can be considered a degenerate case of a four-dimensional polytope and symbolized {4,3,4}. The way to interpret {p,q,r} is that r figures that are {p,q}'s meet at an edge. A space filling by polytopes is often called a *honeycomb* (elsewhere we reserve this term for {6,3})

The four-dimensional simplex is {3,3,3} and the four-dimensional cross polytope is {3,3,4}. There is also a polytope {3,3,5} (which might be thought of as the four-dimensional analog of the icosahedron) whose 600 cells are tetrahedra. Its dual is the regular polytope {5,3,3} (again we might consider this the analog of the dodecahedron) whose 120 cells are dodecahedra. It is noted in passing that the order of the symmetry group of these polyhedra is 14400—this is small for mathematicians but rather impressive compared to the order (48) of the largest three-dimensional crystallographic point group ($m\bar{3}m$) and the order (120) of the icosahedral group.

It transpires that there is a sixth polytope in four dimensions. This is {3,4,3} whose 24 cells are octahedra {3,4} with three meeting at every edge. {3,3,4} and {3,4,3} are space-filling polytopes so there are also four-dimensional honeycombs {3,3,4,3} and {3,4,3,3}.

Only in two and four dimensions are there regular honeycombs other than a space filling by hypercubes. The reader who wants to learn about these beautiful figures can do no better than read the book by Coxeter cited at the end of this appendix.

It is interesting that four dimensions is richest in *regular* polytopes. The geometry of higher dimensions is not dull however, there some remarkable lattices with special properties known. One teaser: the problem of the number of equal spheres that can contact a central one (this is sometimes called the maximum "kissing number") is remarkably difficult to solve. It is known to be 12 in three dimensions, but mathematicians don't know the answer in four dimensions.[1] The maximum kissing number *is* known in 24 dimensions and is 196560; a lattice with this coordination number is also known. The order of the point symmetry group of this lattice is 8315553613086720000 which is *still* small by mathematical standards (the order of the point symmetry group of the primitive hypercubic lattice is $2^n n!$—work *that* out for $n = 24$).

A2.3 Four- and higher-dimensional lattices

In four-dimensions we specify a lattice by four vectors $\mathbf{a}_1$, $\mathbf{a}_2$, $\mathbf{a}_3$, $\mathbf{a}_4$ of length a_1, a_2, a_3, a_4 and with angles between them of α_{12}, α_{13}, α_{14}, α_{23}, α_{24}, α_{34}; i.e., in general, ten unit cell parameters. It transpires that there are 64 Bravais lattices. We look at one or two here. Conceptually the simplest of these is the primitive hypercubic with $a_1 = a_2 = a_3 = a_4 = a$ and all angles equal to 90°. The point symmetry of this lattice is the same as that of the hypercube and has order 384. Each lattice point has 8 neighbors. The primitive hypercubic lattice in n dimensions may be symbolized $\mathbf{Z}^n$.

Recall that in four dimensions the distance from the center to a vertex of a hypercube is equal to an edge length. This means that a copy of the simple hypercubic lattice displaced by 1/2,1/2,1/2,1/2 can be fitted into the first one and generate a new lattice which is known to crystallographers as Z-centered hypercubic (mathematicians know it as D_4). Each point of the new lattice has 24 neighbors. The point at 0,0,0,0 has as neighbors, the original eight of the primitive lattice at (±1,0,0,0)κ and 16 more from the second hypercubic lattice at the vertices of a hypercube with coordinates ±1/2,±1/2,±1/2,±1/2. If spheres of unit radius are put at the lattice points the arrangement with $a = 1$ corresponds to the densest (lattice) packing of spheres in four dimensions. Another way of looking at this lattice is as the vertices of the regular honeycomb {3,3,4,3}. The interstices of the lattice at (1/2,1/2,0,0 ; 1/2,0,1/2,0 ; 1/2,0,0,1/2 ; 0,1/2,1/2,0 ; 0,1/2,0,1/2 ; 0,0,1/2,1/2) are at the centers of the {3,4,3} polytopes.

Now for some vertigo. The positions of the interstices given above are the regular honeycomb {3,4,3,3} and the Voronoi polyhedron of the lattice points is a {3,4,3}. This figure is just the same as that of the 24 lattice points surrounding a given lattice point. In

[1]Mathematicians are hard lot to convince. It is a safe bet that the 24-coordinated lattice described below provides the answer to this problem and that of densest sphere packing in four dimensions. Only recently has it been *proved* that there is not a sphere packing in three dimensions that is denser than cubic closest packing.

fact the point symmetry of the lattice is the same as that of {3,4,3} and is *higher* than that of the primitive hypercubic lattice; the order of the point group is 1152. This means that in four dimensions there are distinct crystal systems corresponding to primitive hypercubic and centered hypercubic.

If we combine the lattice positions (0,0,0,0 ; 1/2,1/2,/12,1/2) with the positions of the interstices (given above) we have eight points which fall back at the points of the same lattice but with separation reduced by a factor of $\sqrt{2}$. In other words we can describe the same lattice using a non-primitive hypercubic unit cell with either 2 points per cell or 8 points per cell. Thus we have two descriptions of the same lattice: (*a*) 0,0,0,0 ; 1/2,1/2,1/2,1/2 ; (*b*) 0,0,0,0 ; 1/2,/12,1/2,1/2 and all six permutations of 1/2,1/2,0,0.

The matrix transforming the first description into the second is:

$$\mathbf{S} = \begin{pmatrix} 1 & 1 & 0 & 0 \\ 1 & -1 & 0 & 0 \\ 0 & 0 & 1 & 1 \\ 0 & 0 & 1 & -1 \end{pmatrix} \qquad \text{(A2.5)}$$

In more than four dimensions there are two distinct lattices, reciprocal to each other, that can be described using a centered hypercubic cell and that are generalizations of the one above. The first, called D_n^*, has lattice points at 0,0,...,0 and 1/2,1/2,... 1/2. The second, called D_n, has lattice points at 0,0,...,0 and all combinations of 0 and 1/2 that add up to an integer. If the coordinates of the points in this second unit cell are doubled, it may be seen that they consist of combinations of integers that add up to an even number, and the lattice points consist of half of the lattice points of a primitive hypercubic lattice; for this reason D_n is also called the checker-board lattice. The unit cell of D_n contains 2^{n-1} points, and for unit distance between lattice points $a = \sqrt{2}$. We have seen that the reciprocal lattice of the *Z*-centered hypercubic lattice (D_4^*) is the same lattice (D_4). Only when $n = 4$ is the point symmetry of D_n different from that of $\mathbf{Z}^n$.

We can't resist mentioning that in eight dimensions two copies of D_8 fit together (in the same way as two primitive hypercubic lattices gave D_4) to give a new lattice E_8. The second D_8 is displaced by 1/4,1/4,...,1/4 from the first. The reader will possibly find it a stimulating exercise to verify that E_8 represents a 240-coordinated sphere packing (the densest known in eight dimensions). For spheres of unit radius, the cell edge remains $\sqrt{2}$ and there are 256 points in the unit cell, i.e. 16 per unit volume. E_8 has attracted some attention in connection with quasicrystal structures; also of interest is that the points divide space into regular simplices and cross polytopes (how many and where?). Note that two D_3 ($\equiv A_3 \equiv fcc$) lattices displaced by 1/4,1/4,1/4 give the diamond structure (not a lattice).

Another family of lattices has non-orthogonal lattice vectors. In a plane we can have three vectors equally inclined to each other at an angle of $\cos^{-1}(-1/2) = 120°$. Two of these of equal length generate a hexagonal lattice. In three-dimensions four vectors all making an equal angle with the others are possible; the angle is the tetrahedral angle, $\cos^{-1}(-1/3) = 109.47°$. Three of these vectors of equal length generate a body-centered cubic lattice (recall that a primitive cell for body-centered cubic has $a = b = c$ and $\alpha = \beta = \gamma = 109.47°$). In

general in n dimensions $n+1$ vectors can be equally inclined at an angle of $\cos^{-1}(-1/n)$ and we can define a lattice using n of them of equal length. Note that the $n + 1$ vectors are equivalent so there will be a symmetry operation of order $n + 1$ relating them as discussed below. The four-dimensional lattice with $a_1 = a_2 = a_3 = a_4 = a$ and $\alpha_{12} = \alpha_{13} = \alpha_{14} = \alpha_{23} = \alpha_{24} = \alpha_{34} = \cos^{-1}(-1/4) = 104.48°$ is known as the primitive icosahedral lattice. The order of the point symmetry group of the lattice is 240.

The lattice reciprocal to this 4-dimensional lattice is easily found to have $a_1 = a_2 = a_3 = a_4 = 1/a$ and $\alpha_{12} = \alpha_{13} = \alpha_{14} = \alpha_{23} = \alpha_{24} = \alpha_{34} = \cos^{-1}(1/2) = 60°$. (Recall that in three dimensions, the lattice reciprocal to *bcc* is the *fcc* lattice which has primitive cell $a = b = c$; $\alpha = \beta = \gamma = 60°$). The simplest way to see this is to find the reciprocal of the **G** matrix:

$$\mathbf{G} = a^2 \begin{pmatrix} 1 & -1/4 & -1/4 & -1/4 \\ -1/4 & 1 & -1/4 & -1/4 \\ -1/4 & -1/4 & 1 & -1/4 \\ -1/4 & -1/4 & -1/4 & 1 \end{pmatrix}$$

$$\mathbf{G}^{-1} = \mathbf{G}^* = a^{-2} \begin{pmatrix} 1 & 1/2 & 1/2 & 1/2 \\ 1/2 & 1 & 1/2 & 1/2 \\ 1/2 & 1/2 & 1 & 1/2 \\ 1/2 & 1/2 & 1/2 & 1 \end{pmatrix} \qquad \text{(A2.6)}$$

The off-diagonal elements of the matrices are $\cos\alpha_{ij}$.

The new lattice can be described using a centered cell of the same shape as the primitive icosahedral lattice and it is then called the *SN*-centered icosahedral lattice. In this description there are 125 lattice points in the (non-primitive) unit cell.

We have remarked that these two lattices are four-dimensional analogs of the *bcc* and *fcc* lattices which, it so happens, are cubic. It is sometimes useful though to consider the *bcc* lattice in terms of its primitive cell. It is left as a non-trivial exercise for the reader to describe the *fcc* lattice in terms of a unit cell with the same shape (it needs 16 points per cell!). The general n-dimensional lattice with primitive cell edges all equal and all angles equal to 60° is known as A_n and its reciprocal lattice with all angles equal to $\cos^{-1}(-1/n)$ is known as A_n^*. A_n represents a lattice sphere packing with $n(n+1)$ neighbors and A_n^* represents a lattice sphere packing with $n + 2$ neighbors.

A2.4 Symmetry operations in four dimensions

It is instructive to see how symmetry operations arise as the dimensionality of space is increased. We restrict ourselves to point symmetry operations (those that leave *at least* one point invariant). In one dimension there is just one operation m that takes a point to another place by reflection in a point. In two dimensions m reflects in a line and in three dimensions

m reflects in a plane. In general m changes position in one direction (the normal to the mirror) and leaves an $n-1$ figure unchanged. Thus in four dimensions there are mirror hyperplanes.

In the transition from one to two dimensions we recognize a new operation that changes two coordinates (leaves a point invariant). The symmetry element is a rotation point. In three dimensions we have a rotation axis (a line is left invariant) and in four dimensions a rotation plane (a plane is left invariant).

Continuing from two to three dimensions, we identify a new operation that changes three coordinates (leaves just a point invariant). This is a (rotation-) inversion point. In four dimensions there are inversion axes[1] and we must seek new symmetry operations that leave only a point invariant. To see their nature it is easiest to appeal to the matrix representations of symmetry operations.

If we use a suitable basis, the matrices representing symmetry operations will always have elements ± 1 and a determinant ± 1 (such matrices are termed *unimodular*). For example an inversion point (at 0,0,0) in three dimensions is represented by the matrix shown below converting x,y,z to $\bar{x},\bar{y},\bar{z}$:

$$\begin{pmatrix} -1 & 0 & 0 \\ 0 & -1 & 0 \\ 0 & 0 & -1 \end{pmatrix} \begin{pmatrix} x \\ y \\ z \end{pmatrix} = \begin{pmatrix} -x \\ -y \\ -z \end{pmatrix} \tag{A2.7}$$

The four-dimensional inversion *axis* (along the w direction) is represented by:

$$\begin{pmatrix} -1 & 0 & 0 & 0 \\ 0 & -1 & 0 & 0 \\ 0 & 0 & -1 & 0 \\ 0 & 0 & 0 & 1 \end{pmatrix} \begin{pmatrix} x \\ y \\ z \\ w \end{pmatrix} = \begin{pmatrix} -x \\ -y \\ -z \\ w \end{pmatrix} \tag{A2.8}$$

An operation that leaves only a point (0,0,0,0) unchanged is:

$$\begin{pmatrix} -1 & 0 & 0 & 0 \\ 0 & -1 & 0 & 0 \\ 0 & 0 & -1 & 0 \\ 0 & 0 & 0 & -1 \end{pmatrix} \begin{pmatrix} x \\ y \\ z \\ w \end{pmatrix} = \begin{pmatrix} -x \\ -y \\ -z \\ -w \end{pmatrix} \tag{A2.9}$$

There are no generally agreed symbols for these symmetry operations, let's call the last one Ξ.[1] It is instructive to break this operation into components.

$$\begin{pmatrix} -1 & 0 & 0 & 0 \\ 0 & -1 & 0 & 0 \\ 0 & 0 & -1 & 0 \\ 0 & 0 & 0 & -1 \end{pmatrix} = \begin{pmatrix} -1 & 0 & 0 & 0 \\ 0 & -1 & 0 & 0 \\ 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & 1 \end{pmatrix} \begin{pmatrix} 1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & -1 & 0 \\ 0 & 0 & 0 & -1 \end{pmatrix} \tag{A2.10}$$

To identify the two matrices on the right we recall that in a three-dimensional Cartesian axis system a two-fold rotation about z is represented as:

$$\begin{pmatrix} -1 & 0 & 0 \\ 0 & -1 & 0 \\ 0 & 0 & 1 \end{pmatrix} \tag{A2.11}$$

so that the first of the two matrices on the right of Eq. A2.10 can be identified as rotation about the zw plane. The second is clearly a rotation about the xy plane. Thus the operation Ξ corresponds to two 2-fold rotations about orthogonal planes (in four dimensions orthogonal planes have only a point on common). It should be obvious that repeating Ξ twice produces the identity, so the order of the operation is 2. It transpires that there are a number of other operations that may be considered as combinations of rotations and that have orders of 3, 4, 6, 8, or 12. The rotations are restricted to 2-, 3-, 4- or 6-fold rotations as in lower dimensions, but the new symmetry operations may have different order.

There is also a 5-fold symmetry operation compatible with translational symmetry in four dimensions. It is instructive to approach it by first considering lower dimensions. A three-fold rotation about a point in two dimensions can be represented by:

$$\mathbf{A} = \begin{pmatrix} 0 & -1 \\ 1 & -1 \end{pmatrix}, \quad \mathbf{A}^2 = \begin{pmatrix} -1 & 1 \\ -1 & 0 \end{pmatrix}, \quad \mathbf{A}^3 = \begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix} \tag{A2.12}$$

In particular this operation takes the point 1,0 to 0,1 to $\bar{1},\bar{1}$ and back to 1,0; i.e. it interchanges the three equivalent axes of a hexagonal lattice.

In three dimensions there is a 4-fold operation that leaves only a point invariant; this is $\bar{4}$. We describe this operation using the basis of a primitive *bcc* cell [i.e. axes inclined at $\cos^{-1}(-1/3)$ to each other]. Successive powers of $\mathbf{A} = \bar{4}$ in this basis are represented by

$$\mathbf{A} = \begin{pmatrix} 0 & 0 & -1 \\ 1 & 0 & -1 \\ 0 & 1 & -1 \end{pmatrix}, \mathbf{A}^2 = \begin{pmatrix} 0 & -1 & 1 \\ 0 & -1 & 0 \\ 1 & -1 & 0 \end{pmatrix}, \mathbf{A}^3 = \begin{pmatrix} -1 & 1 & 0 \\ -1 & 0 & 1 \\ -1 & 0 & 0 \end{pmatrix}, \mathbf{A}^4 = \begin{pmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 1 \end{pmatrix} \tag{A2.13}$$

The nature of $\mathbf{A}$ can be verified (see § 3.7.3) by checking that $\mathrm{Tr}(\mathbf{A}) = -1$ and $\det(\mathbf{A}) = -1$ as well as observing that it has an order of 4. Now the point 1,0,0 is successively taken to

[1]There appears not to be an agreement on the meaning of the word "axis". We use it to mean a one-dimensional figure (straight line) left invariant by a symmetry operation. However one commonly sees the statement that one can have 5-fold symmetry axes in four dimensions; as discussed next the five-fold symmetry operation only leaves a point invariant. The axes in four dimensions are (roto-) inversion axes. The difficulty arises in part because (for example) in three dimensions one needs to specify the direction of the rotation component of a $\bar{4}$ symmetry operation as well as the location of the point of the inversion component even though neither the rotation axis or the inversion point exist separately in this example.

[1]Symbols encountered include 22, 2222, I$\bar{1}$ and $\partial\varepsilon_{22}$.

0,1,0; 0,0,1; $\bar{1},\bar{1},\bar{1}$ and back to 1,0,0. Normally the $\bar{4}$ operation is described using an orthogonal basis so that the matrix representation is different; but of course the trace and determinant of the matrix are unchanged.

Finally coming to four dimensions, there is a five-fold operation that can be represented simply using a basis with axes at $\cos^{-1}(-1/4)$ to each other and which is represented by the matrix **V**:

$$\mathbf{V} = \begin{pmatrix} 0 & 0 & 0 & -1 \\ 1 & 0 & 0 & -1 \\ 0 & 1 & 0 & -1 \\ 0 & 0 & 1 & -1 \end{pmatrix} \qquad \text{(A2.14)}$$

The reader should verify that $\mathbf{V}^5 = \mathbf{E}$ (the unit matrix) and that successive operations on e.g. 1,0,0,0 produce 0,1,0,0 ; 0,0,1,0 ; 0,0,0,1 ; $\bar{1},\bar{1},\bar{1},\bar{1}$ and back to 1,0,0,0. Note that $\det(\mathbf{V}) = 1$, so this is a proper operation. As it transforms a set of integers p,q,r,s representing a lattice point into another set of integers representing another lattice point it is a symmetry element of a lattice and hence compatible with translational symmetry.

Some words of caution. The two-dimensional hexagonal lattice actually has a six-fold symmetry element (6-fold rotation) and the four-dimensional icosahedral lattice has a ten-fold symmetry element (which is a combination of **V** with Ξ [1]) but the three-dimensional lattice does not have an eight-fold symmetry element.[2] The general four-dimensional lattice with a ten-fold symmetry element is referred to as *decagonal*. The unit cell parameter constraints are $a_1 = a_2 = a_3 = a_4$ and $\alpha_{12} = \alpha_{23} = \alpha_{34} = \alpha$, $\alpha_{13} = \alpha_{14} = \alpha_{23} = \beta$, with $\cos\alpha + \cos\beta = -1/2$ (i.e. there are two independent unit cell parameters), we have referred in the previous paragraph to the case $\alpha = \beta$.

To completely identify symmetry operations corresponding to matrices in four dimensions one needs as well as the trace and determinant, the *second invariant* which, for a matrix with elements a_{ij}, is:

$$(a_{11}a_{22} - a_{12}a_{21}) + (a_{11}a_{33} - a_{13}a_{31}) + (a_{11}a_{44} - a_{14}a_{41}) + (a_{22}a_{33} - a_{23}a_{32}) + (a_{22}a_{44} - a_{24}a_{42}) + (a_{33}a_{44} - a_{34}a_{43}) \qquad \text{(A2.15)}$$

Interest in quasicrystals, some of whose *diffraction patterns* have icosahedral symmetry, prompts the observation that in six dimensions, 5-fold "axes" [3] oriented as in icosahedral symmetry are possible (as well as 7-, 9-, 14- and 18-fold symmetry operations).

With orthogonal axes the **V** operation is represented by the matrix:

[1] It should be obvious that just as every three-dimensional *lattice* has $\bar{1}$ for a symmetry element, every four-dimensional lattice has Ξ (which reverses the direction of lattice vectors) as a symmetry element.

[2] A combination of $\bar{4}$ with $\bar{1}$ (*existing separately*) is $4/m$.

[3] See footnote on p. 398.

$$\mathbf{V}' = \begin{pmatrix} \cos\rho_1 & \sin\rho_1 & 0 & 0 \\ -\sin\rho_1 & \cos\rho_1 & 0 & 0 \\ 0 & 0 & \cos\rho_2 & \sin\rho_2 \\ 0 & 0 & -\sin\rho_2 & \cos\rho_2 \end{pmatrix} \qquad \text{(A2.16)}$$

which represents a double rotation first about the zw plane by ρ_1 and then about the xy plane by ρ_2 (compare the discussion of Ξ given above). From the fact the trace must be -1 and the second invariant must be 1 (as for **V**) it can easily be found that $\rho_1 = 2\pi/5$ and that $\rho_2 = 4\pi/5$. Thus the **V** operation is the *combination* of rotations by 1/5 and 2/5 of a circle about orthogonal planes.

A2.5 Numbers of crystallographic symmetry groups

There are 4895 four-dimensional space groups and, as we have seen, the order of the point group can be as high as 1152 so that an *International Tables* for four dimensions with the same detail as Volume *A* (1983) would run to hundreds of volumes, and five dimensions would be out of the question. The table below lists the numbers of crystallographic groups in n dimensions and with lattices of differing ($\leq n$) dimensions of periodicity.

space	lattice dimension →	0	1	2	3	4	n
0		1					
1		2	2				
2		10	7	17			
3		32	75	80	230		
4		227	?	?	1651	4895	
n		?	?	?	?	?	?

The entry under column 0 is the number of crystallographic point groups. It *is* known that the entry in every column is finite for finite n.

A2.6 Generalization of Euler's formula for polyhedra

The generalization to n dimensions of Euler's formula for polyhedra is:

$$\sum_{i=0}^{n-1} (-1)^i P_i = 1 - (-1)^n \qquad \text{(A2.17)}$$

Where P_i is the number of i-dimensional figures (P_0 is the number of vertices, P_1 is the number of edges etc.). For $n = 3$, this gives the familiar formula $P_0 - P_1 + P_2 = 2$ (i.e. $V - E + F = 2$). In four dimensions: $P_0 - P_1 + P_2 - P_3 = 0$. For a four-dimensional

simplex $P_0 = 5$, $P_1 = 10$, $P_2 = 10$, $P_3 = 5$.

From Eq. 2.17 the analogous formula for a honeycomb (space filling by n-dimensional polytopes)can be derived[1]:

$$\sum_{i=0}^{n} (-1)^i P_i = 0 \qquad \text{(A2.18)}$$

Where now the numbers should be interpreted as *relative* numbers of figures of the appropriate dimensionality. For a plane tessellation Eq. A2.18 gives the result: $V - E + F = 0$ which we have used many times. We use the analogous expression for three-dimensional honeycombs in Appendix 3.

A2.7 References

One of the best introductions to elementary n-dimensional geometry is still *An Introduction to the Geometry of n Dimensions* by D. M. Y. Sommerville (Dover, New York, 1958). The definitive work on regular polytopes in n-dimensions is *Regular Polytopes* by H. S. M. Coxeter [third edition, Dover, New York, 1973] and on polytopes in general *Convex Polytopes* by B. Grünbaum [Interscience, New York, 1967]. Four-dimensional lattices are described fully by H. Wondratschek *et al.*, *Acta Crystallogr.* **A27**, 523 (1971) and an account of the four-dimensional space groups is in *Crystallographic Groups of Four-Dimensional Space* by H. Brown *et al.* [Wiley, New York, 1978]. A good introduction to four-dimensional crystallographic point groups and symmetry operations has been given by E. J. W. Whittaker [*An Atlas of Hyperstereograms of the Four-Dimensional Crystal Classes*, Clarendon Press, Oxford, 1985]. The four-dimensional hyperlayer groups (i.e. the symmetry groups of four-dimensional objects with translations in three dimensions) are described in *Colored Symmetry* by A. V. Shubnikov and N. V. Belov [Pergammon Press, Oxford, 1964]. For a wild ride into many-dimensional space (but with some excellent introductory material) *Sphere Packings, Lattices and Groups* [Springer-Verlag (1988)] by J. H. Conway and N. J. A. Sloan is highly recommended (this book also includes an enormous bibliography). There have been many recent examples of higher-dimensional crystallography applied to real world problems a good starting point is T. Janssen, *Acta Crystallogr.* **A42**, 261-271 (1986). Applications to quasicrystals will be found in the review by W. Steurer, *Zeits. Kristallogr.* **190**, 179 (1990). Two commonly used notations for point symmetry operations in four dimensions are those of C. Hermann [*Acta Crystallogr.* **2**, 139-145 (1949)] and A. C. Hurley [*Proc. Cambridge Philos. Soc.* **47**, 650-661 (1951)].

[1]For Eqs. A2.17 and A2.18, see the Coxeter reference cited in the next section.

APPENDIX 3

THE TOPOLOGY OF POLYHEDRA, NETS AND MINIMAL SURFACES

A3.1 Introduction

Topological aspects of crystal chemistry are attracting increasing attention. One reason for the interest is that zeolite catalysts are of major economic importance and their properties are intimately related to structural features such as the size of the pores and cages. These in turn are related to topological properties such as the connectivity and the sizes and numbers of rings in the net of the framework atoms. This Appendix describes some topological aspects of structures, particularly of 3- and 4-connected nets and infinite polyhedra. It will be seen that the subject poses some interesting and challenging unsolved problems.

A3.2 Finite polyhedra

Normally a polyhedron is thought of as a simple convex object topologically equivalent to a sphere: thus if the faces were deformable, it could be "blown up" so that it became a sphere in the same way as a truncated icosahedron (5.6^2) becomes a soccer ball. A finite polyhedron of this sort is topologically equivalent to a tiling of the surface of a sphere. The well-known Euler equation for the number of faces (F), edges (E), and vertices (V) of such a tiling is $F - E + V = 2$

A torus (an object shaped like a doughnut or the inner tube of a tire) has a hole through it, and is topologically different from a sphere. For a tiling of a torus, $F - E + V = 0$. This is the same as for a tiling of the plane (see § 5.6.11).

What about surfaces with more than one hole in them? A teacup with one handle is topologically the same as a torus and contains one hole. A soup bowl with two handles has two holes and is thus topologically distinct. The number of holes in a surface (H) is related to the *Euler-Poincaré characteristic* χ of a surface by:[1]

$$\chi = 2 - 2H \qquad \text{A3.1}$$

and for a surface with characteristic χ:

$$V - E + F = \chi \qquad \text{A3.2}$$

Thus the torus (and the infinite plane) have $\chi = 0$ and a simple closed surface (such as that of a sphere) has $\chi = 2$ ($H = 0$).

[1]See H. S. M. Coxeter, *Introduction to Geometry* (Book List). A simple proof of Eq. A3.2 is given by R. Courant & H. Robbins, *What is Mathematics?* [4th Ed. Oxford (1947)].