(1/2,0,0)κ. Fe has 3 Fe and 3 As neighbors, and As has 4 Fe neighbors. If all edges are equal, $x = 5/\sqrt{2}(\sqrt{6} - 1) = 0.145$ (quite close to the actual value). For the full structure see M. J. Buerger *et al.*, *Zeits. Kristallogr.* **125**, 93 (1967).

(b) An open structure consisting of rings of three tetrahedra (corner sharing) joined by further corner sharing with octahedra occurs in catapleite, $Na_2ZrSi_3O_9.2H_2O$ in which rings of three corner-sharing $\{Si\}O_4$ tetrahedra are joined by $\{Zr\}O_6$ tetrahedra. Data for the non-water atoms are:

catapleite — *P*6$_3$/*mmc*, $a = 7.40$, $c = 10.07$ Å, $V = 477$ Å^3.
Zr in 2 *a*: (0,0,0 ; 0,0,1/2) ; Na in 4 *f*: ± (1/3,2/3,*z* ; 1/3,2/3,1/2+*z*), $z = 0.08$
Si in 6 *h*: ± (x,2x,1/4 ; x,$\bar{x}$,1/4 ; 2$\bar{x}$,$\bar{x}$,1/4), $x = 0.20$; O(1) in 6 *h*, $x = 0.47$
O(2) in 12 *k*: ± (x,2x,z ; x,$\bar{x}$,z ; 2$\bar{x}$,$\bar{x}$,z ; x,2x,z+1/2 ; x,$\bar{x}$,z+1/2 ; 2$\bar{x}$,$\bar{x}$,z+1/2),
$x = 0.135$, $z = 0.125$

In the Zr,Si net, Zr has 6 Si neighbors and Si has 2 Si and 2 Zr neighbors. Not unexpectedly, the Zr-Si distances are rather different (larger) than the Si-Si distances.

(c) A related, but different, structure is found in benitoite, $BaTiSi_3O_9$

benitoite — *P*6̄*c*2, $a = 6.61$, $c = 9.72$ Å, $V = 368$ Å^3
Ba in 2 *f*: (2/3,1/3,0 ; 2/3,1/3,1/2) ; Ti in 2 *c*: (1/3,2/3,0 ; 1/3,2/3,1/2)
Si in 6 *k*: (x,y,1/4 ; $\bar{y}$,x–y,1/4 ; y–x,$\bar{x}$,1/4 ; $\bar{y}$,$\bar{x}$,3/4 ; y–x,y,3/4 ; x,x–y,3/4),
$x = 0.0711$, $y = 0.2894$; O(1) in 6 *k*, $x = 0.2535$, $y = 0.1972$
O(2) in 12 *l*: (as 6 *k* but 1/4 replaced by z and 1/2–z and 3/4 replaced by $\bar{z}$, 1/2+z)
$x = 0.0880$, $y = 0.4302$, $z = 0.1127$

Compare the Zr,Si net in catapleite with the Ti,Si net in benitoite. Note that the latter is much denser (compare the volumes of the unit cells which contain 6 Si atoms in each case).

16. A fascinating open structure based on a 4-connected net is that of the zeolite-like compound: $[N(CH_3)_4]_2MnGe_4S_{10}$ with a framework based on vertex sharing $\{Mn\}S_4$ and $\{Ge\}S_4$ tetrahedra. Ge_4S_{10} "supertetrahedron" units (Fig. 5.18, § 5.2.1) and MnS_4 units are linked as in **diamond** (or better, as in **sphalerite**) so the net of the metal atoms is intermediate between **diamond** and ***D*4**. Here are data for the framework (explore!):

$I\bar{4}$, $a = 9.513$, $c = 14.281$ Å.
Mn in 2 *d*, I + (0,1/2,1/4)
Ge in 8 *g*: I + (x,y,z ; $\bar{x}$,$\bar{y}$,z ; y,$\bar{x}$,$\bar{z}$; $\bar{y}$,x,$\bar{z}$), $x = 0.570$, $y = 0.325$, $z = 0.089$

The vertex symbols are Mn: $9_2{\cdot}9_2{\cdot}9_2{\cdot}9_2{\cdot}9_2{\cdot}9_2$ and Ge: $3{\cdot}9_2{\cdot}3{\cdot}9_2{\cdot}3{\cdot}9_2$.

17. Draw the structure of BeH_2 and show that it is topologically the same as that of moganite (SiO_2).

BeH_2 — *Ibam*, $a = 9.082$, $b = 4.160$, $c = 7.707$ Å ; Be(1) in 4 *a*: I ± (0,0,1/4)
Be(2) in 8 *j*: I ± (x,y,0 ; 1/2–x,1/2+y,0), $x = 0.1699$, $y = 0.1253$
H(1) in 8 *j*, $x = 0.3055$, $y = 0.2823$
H(2) in 16 *k*: I ± (x,y,±z ; 1/2–x,1/2+y,±z), $x = 0.0895$, $y = 0.1949$, $z = 0.1515$

APPENDIX 1

MORE INFINITE SYMMETRY GROUPS

In this appendix we describe some infinite symmetry groups other than the space groups discussed in Chapters 1 and 3. Three-dimensional objects with translational symmetry in only two dimensions are *layers*. The symmetry groups of these objects are the 80 layer groups that are given below. Likewise three-dimensional objects with translational symmetry in only one dimension are *rods*. The 75 crystallographic rod groups are also listed.[1] Two-dimensional objects with one-dimensional translational symmetry are called *bands* or *friezes* and we describe the 7 band groups also.

A convenient way to consider these groups is as derived from space groups by removing translations in one or two dimensions. The reason for doing this is that the coordinates of general and special positions (and their site symmetries), and the nature and location of symmetry elements, can be obtained directly from the space group tables in the *International Tables* (abbreviated here to *IT*). As the coordinates of the general and special positions are the same as those of the space groups from which they are derived, the same labels (Wyckoff notation) are used for them here.

For completeness we also mention the *cylindrical* and *spherical* point groups that describe the symmetries of objects with ∞-fold rotation axes.

A1.1 Layer groups

In the coordinate system used here it is assumed that the translations are along the x and y directions. The lattice can be oblique, either primitive (*p*) or centered (*c*) rectangular, hexagonal or square as for the two-dimensional space groups. The position in the plane group symbol has the same significance as for the three-dimensional space groups.

Once the space group from which the layer group is derived has been identified (and, if necessary, the axes relabeled as explained below) the symmetry elements and their locations and the coordinates of special and general positions are obtained directly from the *IT* (but of course there are no translations along z. In fact z is now to be considered as the height above the $z = 0$ plane, and as such, has dimensions (e.g. z may be measured in Å). The symmetry elements of the layer group are those of the space group which are contained in, or which intersect, the plane $z = 0$.

Comments and examples are taken in order of the system of the corresponding three-dimensional groups. For the full table of groups see § A1.6 (p. 389).

Monoclinic. The cases to be considered are classes 2, *m* and 2/*m*. The 2-fold axis of the layer group can be along z in which case the lattice is oblique. The symbol for the layer

[1]With translations in only one direction, there is no restriction on the nature of rotation axes in rod groups. Here we restrict ourselves to those containing only 1-, 2-, 3-, 4- and 6-fold axes.

group is the same as that for the setting "unique axis *c*" in the *IT*. Only those monoclinic groups with primitive lattices and that do not have screw axes will have layer groups as subgroups in this instance.[1]

If the 2-fold axis of the layer group is parallel to one of the translations, it is taken as the **b** direction and the symbol for the layer group is the same as that for the three-dimensional group in the setting "unique axis *b*" except that (a) the lattice symbol is lower case and (b) the glide direction (if present) must be along **a** (so the glide planes are *a*). The lattice is now rectangular (either *p* or *c*).

It may be seen, for example, that information in the *IT* about $p112/b$ (oblique) and $p12/a1$ (rectangular) are both contained under "nonstandard" settings of number 13, $P12/c1$ ("unique axis *c*, cell choice 3" and "unique axis *b*, cell choice 3" respectively).

Orthorhombic. The cases correspond to classes 222, *mm*2 and *mmm*. Layer glide planes can now be *a* or *b* or, for glide planes in the *xy* plane, *n*. Thus there is a layer group *pban* derived from *Pban*.

Another layer group is $p2_1am$ derived from $P2_1am$, which is a nonstandard setting of $Pmc2_1$ (number 26). Thus to get the information about $p2_1am$, one should first transform $Pmc2_1$ to $P2_1am$. This involves interchanging *x* and *z*. Thus from the *IT* for $Pmc2_1$ we find the general positions: $(\pm x,y,z\ ;\ \pm x,\bar{y},1/2+z)$. For $p2_1am$ the corresponding general positions are: $(x,y,\pm z\ ;\ 1/2+x,\bar{y},\pm z)$ and the symmetry elements of the layer group are those of the space group intersecting, or contained in, the old $x = 0$ (new $z = 0$) plane.

A second layer group derived from $Pmc2_1$ is $p2_1ma$. We first get the general positions of $P2_1ma$ from those of $Pmc2_1$ by cyclic permutation $x \rightarrow y \rightarrow z \rightarrow x$ as: $(x,\pm y,z\ ;\ 1/2+x,\pm y,\bar{z})$. These are also the general positions of $p2_1ma$ and the symmetry elements of the layer group are those of the space group contained in the old $y = 0$ (new $z = 0$) plane.

At the time of writing, there does not appear to be a generally agreed "standard" setting for oblique and rectangular layer groups. Thus, to continue with the same examples, $p2_1am$ could be (and sometimes is) written $pb2_1m$, and $p2_1ma$ could be written $pm2_1b$. In both cases the labels of the *x* and *y* axes have been interchanged.

If in doubt the transformations of axes for different settings of the orthorhombic groups are given on p. 441-442. Note that the last position in the symbol given here for rectangular layer groups *always* refers to the unique direction (normal to the lattice). Layer groups such as *p2mm* and *pmm*2 are distinct groups although they are both derived from *Pmm*2 (number 25). *cmm*2 and *c2mm* are also distinct groups but are now subgroups of two different space groups: *Cmm*2 (number 35) and *C2mm* (a non-standard setting of *Amm*2, number 38). On the other hand *cm2m* is an alternative setting of *c2mm*.

Tetragonal and Hexagonal. The layer groups are derived from the space groups with a primitive lattice that do not have symmetry elements with translational components along *z*. The layer group symbols in these instances are simply derived from the space group symbols by the substitution of *p* for *P*. The positions of the individual entries of the layer group symbol have exactly the same significance as they do for the three-dimensional

[1] Clearly one cannot have symmetry elements that involve translations out of the plane of **a** and **b**.

tetragonal and hexagonal space groups. The symmetry elements of the layer group are now those of the space group contained in, or intersecting $z = 0$.

A1.2 Rod groups

The only one dimensional lattice is primitive and we use the symbol **p** for it.

Many of the remarks of § A1.1 apply also to the rod group symbols. The major difference is that the translational symmetry is along the *z* direction, so symmetry elements with translational components must be along that direction. In particular glide is always *c*.

Note that for tetragonal, trigonal and hexagonal rods the last two positions of the rod group symbol can be interchanged. This is because the orientation of the *x* and *y* axes is not determined by the directions of lattice translations. Thus although $P3m1$ and $P31m$ are different space groups and $p3m1$ and $p31m$ are different layer groups, $\mathbf{p}3m1$ and $\mathbf{p}31m$ are the same rod group with the orientation of *x* and *y* chosen differently (just as $31m$ and $3m1$ are also the same point group). Such redundant rod groups are in parentheses in the Table below (p. 389).

The coordinates of general and special positions are directly available from the *IT*: now *z* is a dimensionless fraction of *c*, and *x* and *y* must be considered to have the dimensions of length. The symmetry elements of the rod group are those of the space group which are on or pass through the line $z = 0$.

A1.3 Examples of layers and rods

There is a large group of layer compounds made up of MX_2 layers of either $\{M\}X_6$ octahedra or $\{M\}X_6$ trigonal prisms sharing edges. The lattices in both cases are hexagonal (Fig. A1.1).

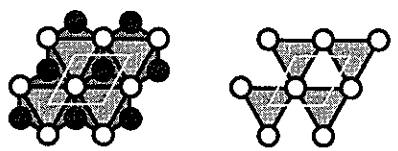

Fig. A1.1. Left part of a layer of MX_6 octahedra. Right part of a layer of MX_6 prisms.

In the octahedral layer *M* is at 0,0,0 and *X* is at $1/3,2/3,z$ and $2/3,1/3,\bar{z}$; these are positions 1 *a* and 2 *d* of $p\bar{3}m1$. The site symmetries are $\bar{3}m$ and $3m$ respectively. In the trigonal prism layer *M* is again at 0,0,0 and *X* is at $2/3,1/3,z$ and $2/3,1/3,\bar{z}$. These are positions 1 *a* and 2 *i* of $p\bar{6}m2$ and the site symmetries are $\bar{6}m2$ and $3m$ respectively.

Another common unit in crystal chemistry is a rod of alternating trigonal prisms and antiprisms (octahedra) sharing triangular faces normal to the rod axis (Fig. A1.2). The

vertices are at $\pm(x,2x,z\ ;\ 2\bar{x},\bar{x},z\ ;\ x,\bar{x},z\ ;\ \bar{x},2\bar{x},1/2+z\ ;\ 2x,x,1/2+z\ ;\ \bar{x},x,1/2+z)$. These are positions 12 *k* of **p**$6_3/mmc$ with site symmetry *m*. The centers of the antiprisms are at 2 *a*: 0,0,0 ; 0,0,1/2 with site symmetry $\bar{3}m$ and the centers of the prisms are at 2 *b*: ± (0,0,1/4) with site symmetry $\bar{6}m2$.

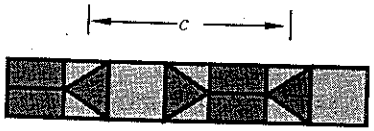

Fig. A1.2. Part of a rod of alternating trigonal prisms and octahedra.

Exercises:

(i) Find *a*, and *z* for the layers of Fig. A1.1 made of regular polyhedra of edge 1 Å.

(ii) Find *x*, *z* and *c* for the rod of Fig. A1.2 made of regular polyhedra of edge 1 Å.

Answers:

(i) $a = 1$ Å, octahedral layer $z = 1/\sqrt{6}$ Å, prism layer $z = 1/2$ Å.

(ii) $x = 1/3$ Å, $z = 1/(4 + \sqrt{24})$, $c = 2 + \sqrt{(8/3)}$ Å. [Note that *x* has dimensions and *z* is dimensionless in Exercise (ii)].

A1.4 One- and two-dimensional "rods" (bands)

In one dimension there are but two point symmetry operations, reflection in a point which we represent by the symbol *m*, and the identity 1. There are therefore, just two point groups: 1 and *m*. Combined with the lattice **p** we get the two one-dimensional space groups **p**1 and **p***m* illustrated below (mirror points are shown as small circles, and the combination of long and short lines, — -, represents an asymmetric object). Note that in **p***m* there are two mirror points per unit cell.

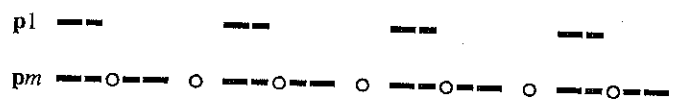

Fig. A1.3. One-dimensional space groups

A two-dimensional object with one-dimensional periodicity is variously referred to as a *band*, *frieze*, or *border*. The symmetry groups of such objects are readily enumerated, and can be related to the two-dimensional space groups just as done above for three-dimensional objects.

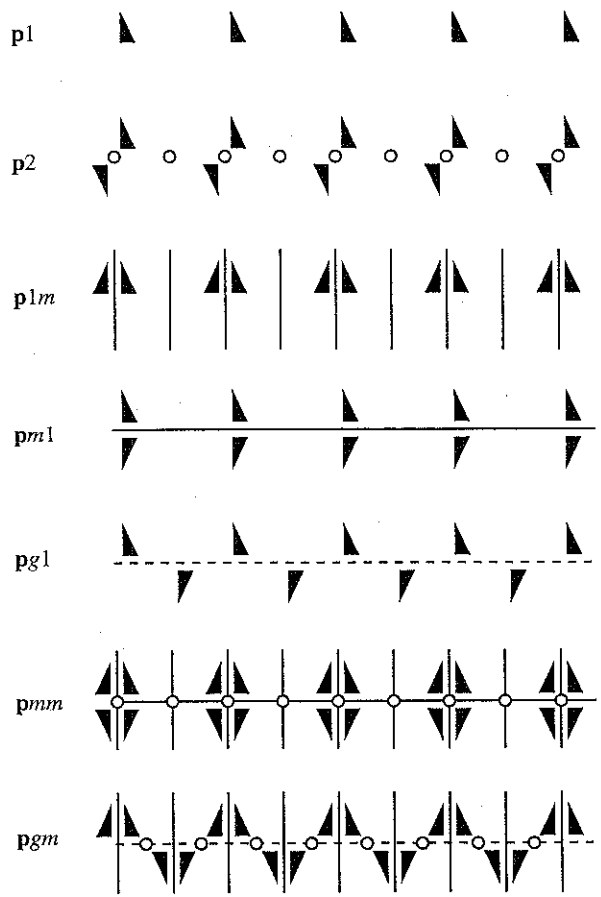

Fig. A1.4. The band groups. In each case the unit cell is the same size. Full lines represent mirror lines and broken lines represent glide lines. Small open circles represent 2-fold rotation points.

The permissible point groups are 1, 2, *m* and *mm*.[1] The first two simply give **p**1 and **p**2. For groups containing mirror lines we must specify their orientations, and we employ Cartesian axes *x* and *y* with the lattice translations along *y*. In accord with the conventions for three-dimensions we take the first position after **p** in the symmetry group symbol to refer to mirror (or glide) lines perpendicular to *x* and the next symbol to refer to mirror lines

[1]It should be obvous that a one-dimensional lattice is not compatible with 3-, 4-, or 6-fold rotation points in the plane containing the lattice.

perpendicular to y. If there is no symmetry element we use "1" as a place marker. Note that a glide line must be along y (perpendicular to x). Thus corresponding to point group m we get band groups $\mathbf{p}m1$, $\mathbf{p}1m$ and $\mathbf{p}g1$. From point group mm we get $\mathbf{p}mm$ and $\mathbf{p}gm$. Patterns with these symmetries (generated by the symmetry elements acting on a scalene triangle) and the symmetry elements are illustrated in Fig. A1.4. Here they are tabulated as in § A1.6:

N	$2D$ groups	band groups
1	$p1$	$\mathbf{p}1$
2	$p2$	$\mathbf{p}2$
3	pm	$\mathbf{p}1m$, $\mathbf{p}m1$
4	pg	$\mathbf{p}g1$
6	pmm	$\mathbf{p}mm$
7	pmg	$\mathbf{p}gm$

N is the number of the space group given in the *IT*. Note that (*a*) in the *IT* the long symbols for the space groups are used. To be consistent with the usage in the *IT* we should write as "long" symbols $\mathbf{p}2mm$ and $\mathbf{p}2gm$ instead of $\mathbf{p}mm$ and $\mathbf{p}gm$. (*b*) for groups $\mathbf{p}m1$ and $\mathbf{p}gm$, x and y have to be interchanged from the setting used in the *IT*.

A1.5 Point groups of infinite order and the symmetry of vectors

In Table 2.4 (§ 2.5.6, p.52) we listed non-crystallographic groups containing a single axis of arbitrary order N. A shortened version of that table is reproduced here using only Hermann-Maugin symbols so we need only consider the cases N even and N odd. We use short symbols for convenience.

$N =$	N	$\bar{N}$	$N2(2)$	$Nm(m)$	N/m	$N/m2/m2/m$	$\bar{N}+m$
$2n$	N	$\bar{N}$	$N22$	Nmm	N/m	N/mmm	$\bar{N}2m$
$2n+1$	N	$\bar{N}$	$N2$	Nm			$\bar{N}m$

There is an interesting relationship between these groups and the band groups. Imagine a finite fragment of the patterns of Fig. A1.4 containing N translations with N even. Now fold the fragment round to make a circle with beginning and end motifs superimposed.[1] If this is done with the pattern of $\mathbf{p}1$, an object of symmetry N is obtained. The same exercise repeated with the $\mathbf{p}2$ pattern will produce symmetry $N22$ (note the two sets of 2-fold axes). Similarly $\mathbf{p}1m$ will produce Nmm (again note the two sets of mirrors), $\mathbf{p}m1$ will produce

[1]The reader who finds the mental exercise difficult is invited to copy Fig. A1.4 and cut the different patterns (which show $N = 4$ translations) into bands, which can then be folded into a ring.

N/m, and $\mathbf{p}mm$ will produce N/mmm. The patterns with glide will probably require a little more thought, but it will be found that $\bar{N}$ is obtained from a fragment of $\mathbf{p}g1$, and $\bar{N}m2$ is obtained from a fragment of $\mathbf{p}gm$. As N gets larger the finite patterns approach the band patterns more and more closely and we can think of the band groups as limiting cases with $N = \infty$ of the point groups with N even. Thus there is a one-to-one correspondence between the band groups and the entries for even N in Table 2.3.

Let us consider the correspondence $Nmm \rightarrow \mathbf{p}1m$ a little further. Fig. A1.5 shows two mirrors inclined at an angle $\alpha = 360°/2N$. Successive reflections in the mirrors generate an N-fold axis at their line of intersection. We can reduce the angle between the mirrors by increasing r and at the same time keeping d constant (see the figure). In the limit $r \rightarrow \infty$ we have parallel mirrors separated by d and successive reflections in these generate a translation by $2d$. Thus the correspondence between point groups and band groups discussed in the previous paragraph is equivalent to considering the infinite set of translations as equivalent to rotations about an axis infinitely far away.

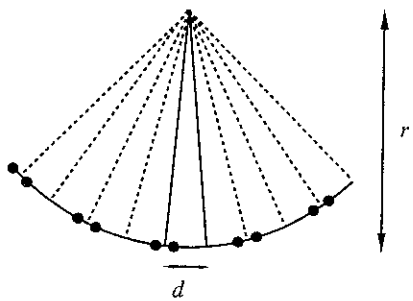

Fig. A1.5. Illustrating the effects of successive reflections in two inclined mirrors (shown as solid straight lines). See the text for details.

There is a second way of reducing the angle between the mirrors. This is by reducing d while keeping r constant; as d goes to zero we will have a finite pattern with an ∞-fold symmetry axis. The symmetry group is now ∞m (only one "m" as it is meaningless to talk of *sets* of mirror planes) and this is the symmetry of, for example, a cone. There are in fact five cylindrical symmetry groups. The reason that there are only five (rather than seven as in the case of the band groups) is that for a finite object with an ∞-fold axis, ∞/m cannot be distinguished from $\bar{\infty}$ (recall that, for example, $\bar{6} \equiv 3/m$). Thus the cylindrical point groups are to be considered as limiting cases as $N \rightarrow \infty$ of the entries in Table 2.3 for N odd. Accordingly the cylindrical groups are:

∞	C_∞	rotating cone
$\bar{\infty} \equiv \infty/m$	$C_{\infty h} \equiv C_{\infty i}$	rotating cylinder or rotating double cone
$\infty 2$	D_∞	antirotating double cone
∞m	$C_{\infty v}$	cone
$\bar{\infty} m \equiv \infty/m2/m$	$D_{\infty d} \equiv D_{\infty h}$	cylinder or double cone

In the table we give the point group symbols (first Hermann-Maugin, then Schoenflies) and then examples of objects with these symmetries. The last two symmetries in the table are realized in linear molecules either without a center of symmetry (as in CO = $C_{\infty v}$) or with one (as in $O_2 = D_{\infty d}$). To realize the first three symmetries we must consider rotating objects. Fig. A1.6 illustrates these. Note that the rotating cone and anti-rotating double cone exist in left- and right-handed (enantiomorphic) forms. In contrast a rotating double cone (or cylinder) has a center of symmetry. The reader who finds this puzzling is asked to look at Fig. A1.6 and then turn the book upside down, and to look at the figure again.[1]

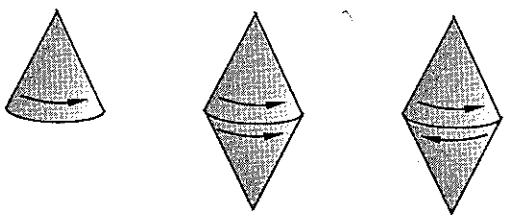

Fig. A1.6. From left to right: a rotating cone, a rotating double cone, and an antirotating double cone.

It is important to recognize that vectors can have one of two symmetries. *Polar* vectors, such as one corresponding to an electric dipole moment have the symmetry (∞m) of a cone. Axial vectors, such as one representing a rotation axis[2] or a magnetic moment have the symmetry ($\bar{\infty}$) of a rotating cylinder. Confusion can arise because it is conventional to represent both kinds of vector by the same symbol—an arrow.[3] As shown in Fig. 1.7 improper operations such as reflection and inversion transform the two kinds of vector differently.

[1]It is useful to recall that the apparent sense of rotation depends on one's point of view. A person looking at a clock will see the hands rotating "clockwise." However from the point of view of the clock, the hands rotate "anticlockwise." Similarly the rotating double cone in the figure is rotating clockwise when viewed from the top but anti-clockwise when viewed from the bottom.

[2]A 2-fold rotation axis is a special case because $2^+ = 2^-$ so the symmetry is $\bar{\infty}m$ and a 2-fold axis does not have a sense (direction). Ironically the symbol for a 2-fold rotation axis in crystallography is an arrow.

[3]See Chapter 1 of *Icons and Symmetry* by S. L. Altmann [Oxford University Press (1992)]. Altmann gives an informative and entertaining account of the Ørsted experiment in which a magnetic needle is deflected by a current flowing in a parallel direction above it. If the magnet and current are both represented by arrows, it appears that the plane containing the magnet and wire is a plane of symmetry. In fact the magnet and current have different symmetries (of axial and polar vectors respectively), and as illustrated in Fig. A1.7, they behave differently on reflection in that plane, which is therefore not really a mirror plane.

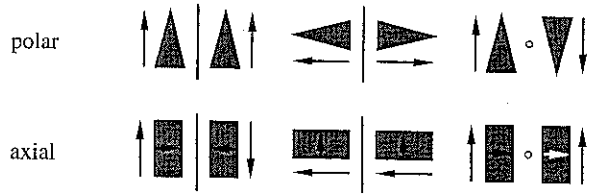

Fig. A1.7. Showing how polar and axial vectors (arrows) and cones and rotating cylinders are transformed by reflection in a mirror (shown as vertical line) and inversion in a center (open circle).

What about groups with more than one N-fold rotation axis? In Chapter 2 we enumerated all the possibilities for finite N. With one ∞-fold axis we get the cylindrical groups. With more than one ∞-fold axis we get the *spherical* groups. A sphere has in fact an infinity of ∞-fold axes and also a center of symmetry so they are actually $\bar{\infty}$ axes. We need at least two to generate spherical symmetry so the symmetry of a sphere is expressed as $\bar{\infty}\,\bar{\infty}$. If the center is removed we get the infinite pure rotation group $\infty\infty$. This second case is hard to imagine: think of a sphere rotating about an axis, and that axis rotating about a second axis at right angles to the first. Thus the spherical groups are (K and K_h are the Schoenflies symbols):

$\infty\infty$	K	rotating sphere
$\bar{\infty}\,\bar{\infty}$	K_h	stationary sphere

In two dimensions the point symmetry groups are N and Nm. If again we let N go to infinity we get the two one-dimensional space groups **p**1 and **p***m* (§ A1.4), and the two infinite point groups (*circular* groups) which are the symmetries of a rotating circle (∞) and of a stationary circle (∞m).

A1.6 Table of layer and rod group symbols

The table on the following pages is intended to be self-explanatory. N is the sequence number in the *IT* of the three-dimensional space groups, which are given in their standard settings. The first page consists of groups with at most 2-fold axes. Then follow groups with 4-fold axes (tetragonal) and groups with 3-fold or 6-fold axes (trigonal and hexagonal)

N	3-D groups	layer groups		rod groups	
	triclinic	oblique			
1	$P1$	$p1$		**p**1	
2	$P\bar{1}$	$p\bar{1}$		**p**$\bar{1}$	
	monoclinic	oblique	rectangular		
3	$P121$	$p112$	$p121$	**p**112	**p**121
4	$P12_11$		$p12_11$	**p**11_1	
5	$C121$		$c121$		
6	$P1m1$	$p11m$	$p1m1$	**p**1*m*	**p**1*m*1
7	$P1c1$	$p11b$	$p1a1$		**p**1*c*1
8	$C1m1$		$c1m1$		
10	$P12/m1$	$p112/m$	$p12/m1$	**p**$112/m$	**p**$12/m1$
11	$P12_1/m1$		$p12_1/m1$	**p**$112_1/m$	
12	$C12/m1$		$c12/m1$		
13	$P12/c1$	$p112/b$	$p12/a1$		**p**$12/c1$
14	$P12_1/c1$		$p12_1/a1$		
	orthorhombic	rectangular			
16	$P222$	$p222$		**p**222	
17	$P222_1$	$p2_122$		**p**222_1	
18	$P2_12_12$	$p2_12_12$			
21	$C222$	$c222$			
25	$Pmm2$	$pmm2$	$p2mm$	**p**$mm2$	**p**$2mm$
26	$Pmc2_1$	$p2_1ma$	$p2_1am$	**p**$mc2_1$	
27	$Pcc2$	$p2aa$		**p**$cc2$	
28	$Pma2$	$pma2$	$p2mb$	**p**$c2m$	
29	$Pca2_1$	$p2_1ab$			
30	$Pnc2$	$p2an$			
31	$Pmn2_1$	$p2_1mn$			
32	$Pba2$	$pba2$			
35	$Cmm2$	$cmm2$			
38	$Amm2$	$c2mm$			
39	$Abm2$	$c2mb$			
47	$Pmmm$	$pmmm$		**p**mmm	
49	$Pccm$	$pmaa$		**p**ccm	
50	$Pban$	$pban$			
51	$Pmma$	$pmma$	$pmam$	**p**mcm	
53	$Pmna$	$pbmn$			
54	$Pcca$	$pbaa$			
55	$Pbam$	$pbam$			
57	$Pbcm$	$pmab$			
59	$Pmmn$	$pmmn$			
65	$Cmmm$	$cmmm$			
67	$Cmma$	$cmma$			

Tetragonal (square) layer and rod groups

N	3-D group	layer group	rod group
75	$P4$	$p4$	**p**4
76	$P4_1$		**p**4_1
77	$P4_2$		**p**4_2
78	$P4_3$		**p**4_3
81	$P\bar{4}$	$p\bar{4}$	**p**$\bar{4}$
83	$P4/m$	$p4/m$	**p**$4/m$
84	$P4_2/m$		**p**$4_2/m$
85	$P4/n$	$p4/n$	
89	$P422$	$p422$	**p**422
90	$P42_12$	$p42_12$	
91	$P4_122$		**p**4_122
93	$P4_222$		**p**4_222
95	$P4_322$		**p**4_322
99	$P4mm$	$p4mm$	**p**$4mm$
100	$P4bm$	$p4bm$	
101	$P4_2cm$		**p**4_2cm
103	$P4cc$		**p**$4cc$
111	$P\bar{4}2m$	$p\bar{4}2m$	**p**$\bar{4}2m$
112	$P\bar{4}2c$		**p**$\bar{4}2c$
113	$P\bar{4}2_1m$	$p\bar{4}2_1m$	
115	$P\bar{4}m2$	$p\bar{4}m2$	[**p**$\bar{4}m2 \equiv$ **p**$\bar{4}2m$]
117	$P\bar{4}b2$	$p\bar{4}b2$	
123	$P4/mmm$	$p4/mmm$	**p**$4/mmm$
124	$P4/mcc$		**p**$4/mcc$
125	$P4/nbm$	$p4/nbm$	
127	$P4/mbm$	$p4/mbm$	
129	$P4/nmm$	$p4/nmm$	
131	$P4_2/mmc$		**p**$4_2/mmc$

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	$P3_221$		$\mathbf{p}3_221$
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 $\pm(b/\sqrt{2}, 0, \ldots 0)\kappa$. 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 $(0,0,\ldots,0)$ and with radius r are given by:

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