The 80 Diperiodic Groups in Three Dimensions

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The low-energy electron diffraction work of L. H. Germer, J. J. Lander, A. U. MacRae, J. Morrison and others is resulting in new information about surface structures. These three-dimensional structures have periodicity only in two dimensions. The 230 triperiodic space groups are not applicable to the solution of these structures. The 17 strictly two-dimensional groups do not admit the existence of a third dimension and may therefore not be appropriate for these structures which are not strictly planar. The useful space groups for these structures are the 80 diperiodic groups in three dimensions.

Nowhere in the literature have these been put into a form convenient for use, as have the other two sets of space groups. This has now been done and the tables are available on request from the Circulation Manager, Bell System Technical Journal, Bell Telephone Laboratories, Incorporated, 463 West Street, New York 14, N. Y. Sample tables are given in this paper.

I. BACKGROUND

Crystals grown under favorable conditions acquire an external shape whose symmetry has long attracted attention. Nineteenth century mineralogists systematically described the symmetry of these shapes in terms of *symmetry operations*. For example, the operation of *rotation* of a cube through 90° around an axis normal to a cube face brings the cube into a position indistinguishable from its original position. An operation that achieves this indistinguishability is called a symmetry operation. In this example the cube will present an identical appearance four times during a rotation of 360° around the axis, which is therefore called "an axis of 4-fold symmetry" or simply "a 4-fold axis." A cube has three 4-fold axes, four 3-fold axes (corner-to-corner) and six 2-fold axes (mid-edge-to-mid-edge) (Figs. 1a and b). Such axes are called *symmetry elements*. The terms "tetrad," "triad" and "diad" are also used for them.

Another type of symmetry element is a mirror plane, across which the operation of *reflection* produces an object indistinguishable from the original. Such a plane through the center of a cube parallel to two opposite faces reflects the left half into the right half and vice versa; that is, the two halves are mirror images of each other. Since there are also diagonal mirror planes in a cube there is a total of nine planes (Figs. 1c and d).

There is also a *center* of symmetry in the center of a cube which relates any feature located a given distance from it in one direction to an indistinguishable feature located the same distance away in the opposite direction. The operation is called *inversion*.

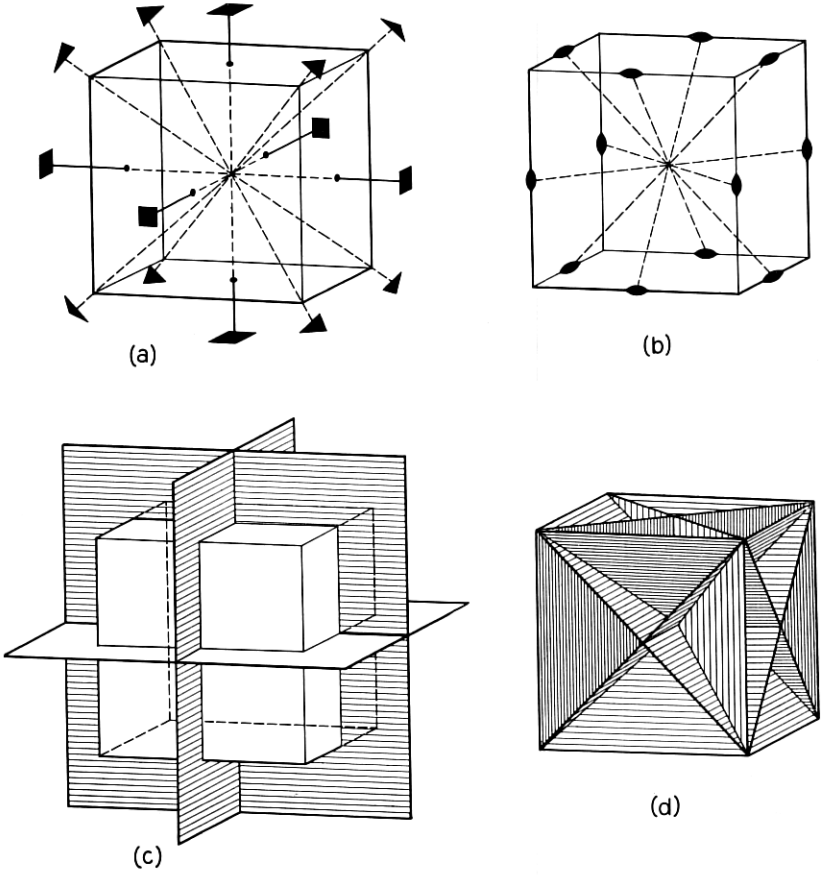


Fig. 1 — The symmetry elements of a cube: (a) the three 4-fold axes and the four 3-fold axes, (b) the six 2-fold axes, (c) three mirror planes parallel to the faces, and (d) six diagonal mirror planes.

An *inversion axis* combines the operation of rotation with that of inversion. The familiar regular tetrahedron which has neither a 4-fold axis nor a center of symmetry has a 4-fold inversion axis because after a rotation of 90° *plus* an inversion through the center point it occupies a position in space indistinguishable from its original position. A center of symmetry is equivalent to a one-fold inversion axis.

Note that during the entire group of "operations" on the cube, one point (the center of the cube) remains unmoved. Another way of saying this is to say that all of the symmetry elements pass through a single point. This group of operations or the symmetry elements which represent them therefore constitute the point group symmetry of the cube. When similar groups of operations are determined for all possible crystals, it is found that there are only 32 possible crystallographic point groups.

The symmetry of shape is the outward expression of the inner orderly atomic arrangement of the crystal. Any property of any piece of the crystal must obey the point group symmetry even though the piece be a ground sphere a few tenths of a millimeter in diameter.

When we consider in detail the *crystal structure* — that is, the positions of the atoms relative to each other — we find that the symmetry elements occur at well-defined positions in space and do not all go through the same point. This is readily illustrated by Fig. 2, the projection of the structure of calcite ($CaCO_3$) onto a plane normal to its 3-fold symmetry axis. Note that the 3-fold axis cannot be randomly placed, normal to the paper, but must pass through the black spots representing the carbon atoms, and further that there is a 3-fold axis through every carbon atom. There are also mirror planes in calcite. We could make a 3-dimensional model of the array of symmetry elements of calcite, and the operation of any symmetry element would shift every other symmetry element to a position indistinguishable from its original position.

Such a self-consistent array of symmetry elements in space is called a *space group*. Since location in space (not orientation alone) is of significance here, two other kinds of symmetry operations become meaningful: operations which combine *translation* with either rotation or reflection. The resulting symmetry elements are called, respectively, *screw axes* and *glide planes*.

As in the case of point groups, the space groups are limited in number. There are 230 possible space groups, i.e., 230 possible self-consistent arrangements in space of all the symmetry elements mentioned above.

Diagrams of these are given in the International Tables for X-ray Crystallography (edited by Henry and Lonsdale, 1952; see References).

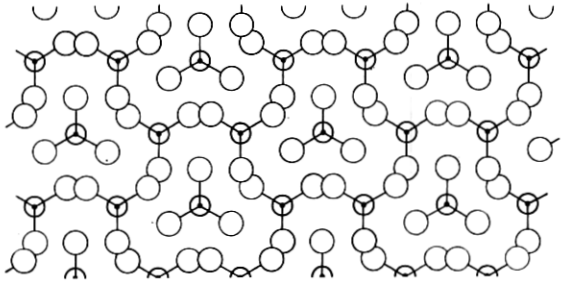


Fig. 2 — The structure of calcite projected onto a plane normal to its 3-fold symmetry axis.

The one appropriate to the structure of calcite is shown on the next page.* It is identified by the symbol $R\bar{3}c$ which states that the unit cell (the repeat unit of the structure) is rhombohedral in shape (R), that it has a 3-fold inversion axis ($\bar{3}$) with a glide plane parallel to it in which the translation is in the c direction.† Of course the 3-fold axis operating on this glide plane generates two more. Additional symmetry elements which are found to exist whenever the stated symmetry operations are performed are also shown in the calcite space group diagram.

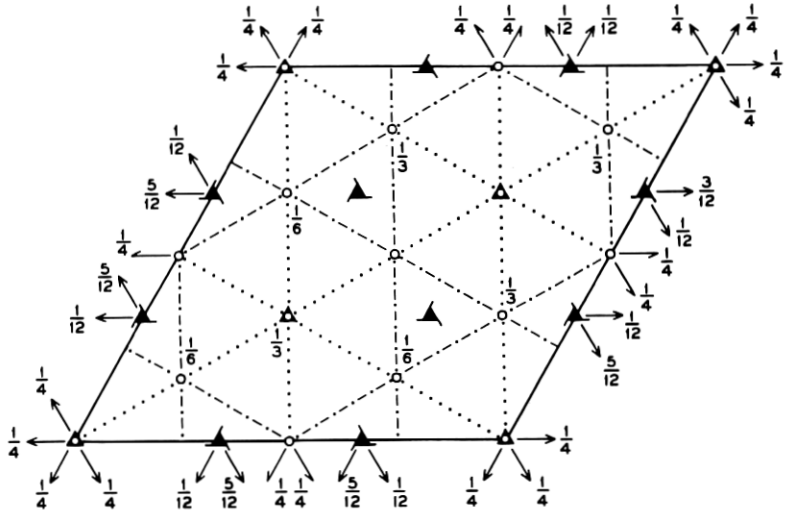
The space group of a crystal can in many cases be uniquely determined directly from x-ray diffraction data. Since, in any given space group, the possible atom positions will be related in a well defined manner by the symmetry operations, a knowledge of the space group is a very powerful aid in determining the arrangement of atoms in the crystal, i.e., the crystal structure.

One could repetitiously extend the space-group symbols in the diagram, as we have the calcite structure in Fig. 2, by translation which would be in three dimensions if we were not limited to the printed page. (The translation vectors define the edges of the *unit cell*, the repeat unit of the three-dimensional structure.) The three-dimensional lattice of translation vectors which would represent this operation is called a *space lattice*. There are only 14 such lattices possible.

If we limit our attention strictly to two dimensions we find that, instead of 230 space groups, we have 17 *plane groups* and instead of 14 space lattices we have 5 *nets*. Here the periodicity no longer extends in three dimensions (triperiodicity) but only in two dimensions (diperiodicity).

* Fractions on the diagram refer to positions of symmetry elements along the c direction (normal to the paper). The unit is the unit length of c, i.e., the c dimension of the unit cell.

† For a very brief discussion of space group symbols see the *Crystallographic Data* section of the American Institute of Physics Handbook.



Symbols of Symmetry Planes

Symbol	Symmetry plane	Graphical symbol: Normal to plane of projection	Nature of glide translation
c	Axial glide plane	.....	$c/2$ along z-axis; or $(a+b+c)/2$ along [111] on rhombohedral axes.
n	Diagonal glide plane (net)	-·-·-·-·-	$(a+b)/2$ or $(b+c)/2$ or $(c+a)/2$; or $(a+b+c)/2$ (tetragonal and cubic).

Symbols of Symmetry Axes

Symbol	Symmetry axis	Graphical symbol	Nature of right-handed screw translation along the axis	Symbol	Symmetry axis	Graphical symbol	Nature of right-handed screw translation along the axis
1	Rotation monad	None	None	2_1	Screw diad	(normal to paper)	$c/2$
$\bar{1}$	Inversion monad	o	None			(parallel to paper)	$a/2$ or $b/2$ or $(a+b)/2$
2	Rotation diad	(normal to paper)	None			Normal to paper	
		(parallel to paper)		3	Rotation triad	▲	None
				3_1	Screw triads	▲	$c/3$
				3_2		▲	$2c/3$
				$\bar{3}$	Inversion triad	△	None

It is with still a third set of groups, the 80 diperiodic groups in three dimensions, that the present paper is concerned.

II. DISCUSSION OF THE 80 DIPERIODIC GROUPS

The International Tables for X-ray Crystallography (1952) ("ITXRC") give two different sets of space groups: the familiar 230 triperiodic space groups and the 17 two-dimensional space groups in which all operations are confined strictly to two dimensions. In the latter set, any operation which admits the existence of the third dimension, such as a two-fold axis lying in the plane, is forbidden.

The existence of a set of groups which admit such operations, but still refer to arrays that are infinitely periodic in only two dimensions, was recognized by several authors at about the same time (Speiser, 1927; C. Hermann, 1928; Alexander and K. Herrmann, 1928; L. Weber, 1929; Alexander and K. Herrmann, 1929). These and subsequent authors (see references at end of this paper) have used a wide variety of nomenclature, some giving some diagrams. C. Hermann gives point positions, but in many cases chooses a different origin and in some cases a larger cell than that given in ITXRC. This work and others contain errors and omissions and none of the authors has given the groups in the form currently used in the International Tables so that they could be conveniently used for structure determination. This has now been done.

Consideration of the restrictions imposed by the loss of periodicity in the third dimension leads to the exclusion of the following symmetry elements: (*i*) screw axes normal to the plane of diperiodicity, (*ii*) glide planes with glide directions out of this plane, and (*iii*) n-fold axes not normal to this plane, with $n > 2$. Since the upper side of our diperiodic array may be like or unlike the lower side, mirror planes, glide planes, two-fold rotation and screw axes may lie in the plane.

It is possible to choose the 80 diperiodic groups in three dimensions from the pages of the existing International Tables for X-ray Crystallography by using some of the "1st setting" monoclinic groups and some of the "2nd setting" monoclinic groups as well as various orientations of the orthorhombic groups, without deletion or addition of any symmetry operations. In the diperiodic-group case we always have a unique direction in the plane-normal. Placing this direction along each of two nonequivalent directions in a single (orthorhombic) triperiodic space group gives us two nonequivalent diperiodic groups. This, of course, requires the appropriate permutation of point coordinates and indices of forbidden reflections.

Special positions of atoms with a fixed coordinate expressed as a frac-

tion of the unit-cell length in the z-direction, other than zero, are not allowed since fractions of a period are meaningless in this nonperiodic direction.

The five nets (comparable to the 14 space lattices in three dimensions) for these diperiodic groups are the same as those for the 17 two-dimensional groups, namely, oblique ($a \neq b$, $\gamma \neq 90°$), primitive and centered rectangular ($a \neq b$, $\gamma = 90°$), square ($a = b$, $\gamma = 90°$), and hexagonal ($a = b, \gamma = 120°$), where γ is the angle between the a and b axes.

Alexander and Herrmann became interested in these groups because of their work with the smectic state in liquid crystals where only two-dimensional periodicity obtains. Cochran's interest in them grew out of his use of "generalized crystal-structure projections" (Cochran, 1952, b) and Holser's (1958, b) out of his investigation of the structure at the boundary between two parts of a twinned crystal (1958, a).

The interest of the writer in making these groups available in convenient form stems from cooperation with those members of Bell Laboratories who have been investigating surface structures by means of low-energy electron diffraction, in particular, L. H. Germer, J. J. Lander, A. U. MacRae and J. Morrison.* These structures are infinitely periodic in two dimensions but lack periodicity in the third dimension (normal to the surface).

Which set of diperiodic groups is appropriate for surface structures? Certainly the structures are not strictly planar: the atoms of the surface structure in many cases do not all lie in the same plane. But would an atom above some plane (parallel to the surface) be symmetrically related to an atom on the other side of the plane? Strictly speaking the atoms could not be symmetrically equivalent since one is closer to the substrate than the other and is therefore in a different force field. From this point of view one would say that only the seventeen strictly two-dimensional space groups would be useful. However, it is frequently so, in triperiodic crystallography, that the symmetry of a crystal structure closely approximates a symmetry that is higher than its true symmetry and that the use of the higher-symmetry space group is of great help in determining the structure. From this point of view one would say that the 80 diperiodic groups in three dimensions are likely to be useful in the solution of diperiodic surface structures. Their application to this field was suggested to the writer by A. L. Patterson.

There follow (*i*) a summary table, Table I; (*ii*) a diagram of net types, Fig. 3; (*iii*) an explanation of terms and symbols used in the

* For a survey of some of this work, see Low-energy Electron Diffraction, by A. U. MacRae, Science, **139**, 1963, pp. 379–388.

TABLE I—SUMMARY TABLE OF THE 80 DIPERIODIC GROUPS IN THREE DIMENSIONS

Net	Diperiodic Group (DG) Number	Full Hermann-Mauguin Symbols	Triperiodic-Group Schoenflies Symbol, ITXRC Number and Orientation, if other than that given in ITXRC		Symbol Proposed by A. Niggli	Weber Number*
Oblique	1	$P1$	C_1^1 - 1		$1P1$	1
	2	$P\bar{1}$	C_i^1 - 2		$1P\bar{1}$	2
	3	$P211$	C_2^1 - 3	1st setting	$1P2$	8
	4	$Pm11$	C_s^1 - 6	1st setting	$mP1$	3
	5	$Pb11$	C_s^2 - 7	1st setting	$aP1$	4
	6	$P2/m\ 11$	C_{2h}^1 - 10	1st setting	$mP2$	12
	7	$P2/b\ 11$	C_{2h}^4 - 13	1st setting	$aP2$	13
Rectangular	8	$P112$	C_2^1 - 3	2nd setting	$1P12$	9
	9	$P112_1$	C_2^2 - 4	2nd setting	$1P12_1$	10
	10	$C112$	C_2^3 - 5	2nd setting	$1C12$	11
	11	$P11m$	C_s^1 - 6	2nd setting	$1P1m$	5
	12	$P11a$	C_s^2 - 7	2nd setting $\bar{c}ba$	$1P1g$	6
	13	$C11m$	C_s^3 - 8	2nd setting	$1C1m$	7
	14	$P11\ 2/m$	C_{2h}^1 - 10	2nd setting	$1P12/m$	14
	15	$P11\ 2_1/m$	C_{2h}^2 - 11	2nd setting	$1P12_1/m$	15
	16	$C11\ 2/m$	C_{2h}^3 - 12	2nd setting	$1C12/m$	16
	17	$P11\ 2/a$	C_{2h}^4 - 13	2nd setting $\bar{c}ba$	$1P12/g$	18
	18	$P11\ 2_1/a$	C_{2h}^5 - 14	2nd setting $\bar{c}ba$	$1P12_1/g$	17
	19	$P222$	D_2^1 - 16		$1P222$	33
	20	$P222_1$	D_2^2 - 17	bca	$1P222_1$	34
	21	$P22_12_1$	D_2^3 - 18		$1P22_12_1$	35
	22	$C222$	D_2^6 - 21		$1C222$	36
	23	$P2mm$	C_{2v}^1 - 25		$1P2mm$	19
	24	$Pmm2$	C_{2v}^1 - 25	bca	$mP12m$	23
	25	$Pm2_1a$	C_{2v}^2 - 26	$\bar{c}ba$	$mP12_1g$	24
	26	$Pbm2_1$	C_{2v}^2 - 26	$a\bar{c}b$	$aP12_1m$	25
	27	$Pbb2$	C_{2v}^3 - 27	$a\bar{c}b$	$aP12g$	26
	28	$P2ma$	C_{2v}^4 - 28		$1P2mg$	20
	29	$Pam2$	C_{2v}^4 - 28	$a\bar{c}b$	$bP12m$	27
	30	$Pab2_1$	C_{2v}^5 - 29	$a\bar{c}b$	$bP12_1g$	28
	31	$Pnb2$	C_{2v}^6 - 30	bca	$nP12g$	29
	32	$Pnm2_1$	C_{2v}^7 - 31	$a\bar{c}b$	$nP12_1m$	30
	33	$P2ba$	C_{2v}^8 - 32		$1P2gg$	21
	34	$C2mm$	C_{2v}^{11} - 35		$1C2mm$	22
	35	$Cmm2$	C_{2v}^{14} - 38	bca	$mC12m$	31
	36	$Cam2$	C_{2v}^{15} - 39	bca	$aC12m$	32
	37	$P2/m\ 2/m\ 2/m$	D_{2h}^1 - 47		$mP2mm$	37
	38	$P2/a\ 2/m\ 2/a$	D_{2h}^9 - 49	cab	$aP2mg$	38
	39	$P2/n\ 2/b\ 2/a$	D_{2h}^4 - 50		$nP2gg$	39
	40	$P2/m\ 2_1/m\ 2/a$	D_{2h}^5 - 51	$a\bar{c}b$	$mP2mg$	40
	41	$P2/a\ 2_1/m\ 2/m$	D_{2h}^5 - 51		$aP2mm$	41
	42	$P2/n\ 2/m\ 2_1/a$	D_{2h}^7 - 53	$a\bar{c}b$	$nP2mg$	42
	43	$P2/a\ 2/b\ 2_1/a$	D_{2h}^8 - 54	cab	$aP2gg$	43
	44	$P2/m\ 2_1/b\ 2_1/a$	D_{2h}^9 - 55		$mP2gg$	44
	45	$P2/a\ 2_1/b\ 2_1/m$	D_{2h}^{11} - 57	bca	$aP2gm$	45
	46	$P2/n\ 2_1/m\ 2_1/m$	D_{2h}^{13} - 59		$nP2mm$	46
	47	$C2/m\ 2/m\ 2/m$	D_{2h}^{19} - 65		$mC2mm$	47
	48	$C2/a\ 2/m\ 2/m$	D_{2h}^{21} - 67		$aC2mm$	48
Square	49	$P4$	C_4^1 - 75		$1P4$	58
	50	$P\bar{4}$	S_4^1 - 81		$1P\bar{4}$	57
	51	$P4/m$	C_{4h}^1 - 83		$mP4$	61
	52	$P4/n$	C_{4h}^3 - 85		$nP4$	62
	53	$P422$	D_4^1 - 89		$1P422$	67
	54	$P42_12$	D_4^2 - 90		$1P42_12$	68
	55	$P4mm$	C_{4v}^1 - 99		$1P4mm$	59

TABLE I—CONTINUED

Net	Diperiodic Group (DG) Number	Full Hermann-Mauguin Symbols	Triperiodic-Group Schoenflies Symbol ITXRC Number and Orientation, if other than that given in ITXRC	Symbol Proposed by A. Niggli	Weber Number*
Square (cont.)	56	$P4bm$	C_{4v}^{2} - 100	$1P4gm$	60
	57	$P\bar{4}2m$	D_{2d}^{1} - 111	$1P\bar{4}2m$	63
	58	$P\bar{4}2_1m$	D_{2d}^{3} - 113	$1P\bar{4}2_1m$	64
	59	$P\bar{4}m2$	D_{2d}^{5} - 115	$1P\bar{4}m2$	65
	60	$P\bar{4}b2$	D_{2d}^{7} - 117	$1P\bar{4}g2$	66
	61	$P4/m\ 2/m\ 2/m$	D_{4h}^{1} - 123	$mP4mm$	69
	62	$P4/n\ 2/b\ 2/m$	D_{4h}^{3} - 125	$nP4gm$	70
	63	$P4/m\ 2_1/b\ 2/m$	D_{4h}^{5} - 127	$mP4gm$	71
	64	$P4/n\ 2_1/m\ 2/m$	D_{4h}^{7} - 129	$nP4mm$	72
Hexagonal	65	$P3$	C_{3}^{1} - 143	$1P3$	49
	66	$P\bar{3}$	C_{3i}^{1} - 147	$1P\bar{3}$	50
	67	$P312$	D_{3}^{1} - 149	$1P312$	54
	68	$P321$	D_{3}^{2} - 150	$1P321$	53
	69	$P3m1$	C_{3v}^{1} - 156	$1P3m1$	51
	70	$P31m$	C_{3v}^{2} - 157	$1P31m$	52
	71	$P\bar{3}1\ 2/m$	D_{3d}^{1} - 162	$1P\bar{3}1m$	55
	72	$P\bar{3}\ 2/m\ 1$	D_{3d}^{3} - 164	$1P\bar{3}m1$	56
	73	$P6$	C_{6}^{1} - 168	$1P6$	76
	74	$P\bar{6}$	C_{3h}^{1} - 174	$mP3$	73
	75	$P6/m$	C_{6h}^{1} - 175	$mP6$	78
	76	$P622$	D_{6}^{1} - 177	$1P622$	79
	77	$P6mm$	C_{6v}^{1} - 183	$1P6mm$	77
	78	$P\bar{6}m2$	D_{3h}^{1} - 187	$mP3m2$	74
	79	$P\bar{6}2m$	D_{3h}^{3} - 189	$mP32m$	75
	80	$P6/m\ 2/m\ 2/m$	D_{6h}^{1} - 191	$mP6mm$	80

* Useful for cross-comparison of this list with those of Weber (1929), C. Hermann (1928) and Alexander and Herrmann (1929) since the equivalence among these three is given in the last reference.

tables, Table II; (*iv*) samples of the systematic ITXRC "tables" for the 80 diperiodic groups in three dimensions, adapted from the three-dimensional space groups by making the appropriate modifications; and (*v*) an annotated list of references.

The full set of 80 diperiodic groups in three dimensions has been bound separately and is available from the Circulation Manager, Bell System Technical Journal, Bell Telephone Laboratories, Incorporated, 463 West Street, New York 14, N. Y. It is anticipated that these groups will be included in a later volume of the International Tables.

III. TABLES OF THE 80 DIPERIODIC GROUPS IN THREE DIMENSIONS

In the sample tables, the usage and notation of the International Tables for X-ray Crystallography for the three-dimensional space groups have been followed as closely as possible. Chosen directly from the

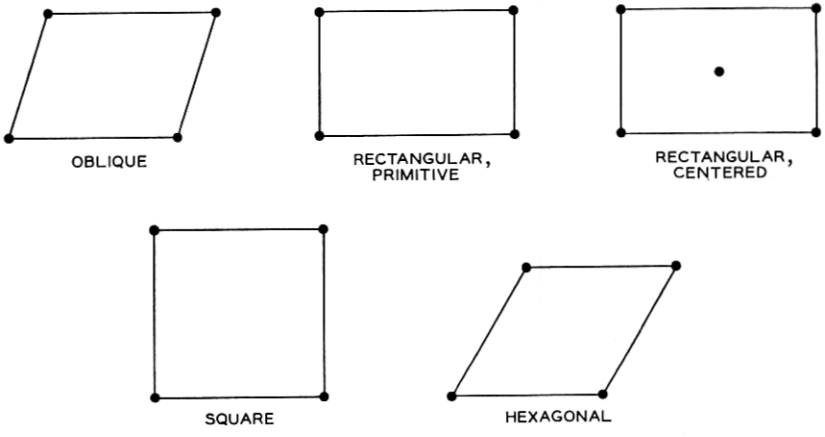


Fig. 3 — The five nets.

ITXRC Tables for the 230 space groups, these tables carry the same atom-position lettering. Letters of forbidden positions will therefore be missing.

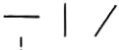
In the oblique and rectangular system, the ITXRC convention of listing the symmetry symbols in the order a, b, c has not been retained. Holser (1958,b) chose to permute these so that the first symbol referred to the c axis. The justification for this is that in the plane groups the c axis is unique and therefore should be put first as in, for example, the tetragonal system (e.g., $4mm$).

The possibility of confusion with the 230 three-dimensional groups will probably be avoided in all cases by the context. However, to aid in the distinction, the plane groups have been numbered, DG1, DG2, etc. The same letters could be used to distinguish DG$Pmm2$, for example, from the three-dimensional C_{2v}^1 - $Pmm2$, but since, in all cases, the two groups do in fact comprise the same symmetry operations, such a distinction may be undesirable.

The order of the DG list is that of the ITXRC which, in turn, is the Schoenflies order.

After this paper was in galley form a communication was received from A. Niggli to whom a manuscript copy had been sent. Niggli favors placing before the lattice symbol (P or C) that symbol referring to the glide plane or mirror plane which lies in the plane of diperiodicity and therefore occurs only once. This occurs in 37 of the 80 groups. This would be another way of distinguishing these groups from the triperiodic groups. The symbol proposed by Niggli is also listed in Table I.

TABLE II — SYMBOLS USED IN THE 80 DG TABLES

Symmetry Elements	Diperiodic Group Symbol	Symbol in the Symmetry Diagram	
		Normal to the Paper	Parallel to the Paper
mirror	m		
glide plane*	a		
	b		
	n	not allowed	
2-fold rotation axis	2		
3-, 4- and 6-fold rotation axes	3, 4, 6		not allowed
2-fold screw axis	2_1	not allowed	
center of symmetry	$\bar{1}$		
3-, 4- and 6-fold inversion axes†	$\bar{3}$, $\bar{4}$, $\bar{6}$		not allowed
Center, on 2-fold axis			

* This operation combines reflection with translation of $\frac{1}{2}$ the length of the cell in the direction indicated by the letter. The diagonal glide, n, combines reflection with translation of $\frac{1}{2}$ of the length of the cell in both the a and b directions.

† Combined rotation through $360°/n$ (for $\bar{n}$) and inversion. Not equivalent to the two operations performed separately.

IV. EXPLANATION OF TERMS AND SYMBOLS USED ON THE 80 DG SHEETS

(These are the same as those used in the ITXRC)

1. *Top of sheet, left to right:* Net-type, full Hermann-Mauguin diperiodic group symbol, diperiodic-group (DG) number. The Hermann-Mauguin symbol begins with a letter which indicates whether the net is primitive or centered and is followed by symbols for symmetry elements that relate to the c, a and b axis, in turn. The c axis is normal to the paper in the diagrams, the a axis is directed toward the bottom of the page, and the b axis is directed toward the right. In DG 46 ($P\ 2/n\ 2_1/m\ 2_1/m$), for example, the lattice is primitive, there is a two-fold axis parallel to c with a diagonal-glide plane normal to c, a two-fold screw axis parallel to a with a mirror plane normal to a, and a two-fold screw axis parallel to b with a mirror plane normal to b. In DG 16 ($C\ 11\ 2/m$) we have a centered net with a two-fold axis parallel to b and a mirror plane normal to b.

2. *Diagrams:* On the right, the distribution of the symmetry elements in the unit mesh. On the left, the distribution in the unit mesh of the points in the "general position" (x, y, z and points symmetrically

equivalent to it). Here, the value of x is taken, arbitrarily, to be a very small distance and y, a slightly larger distance, except in the oblique groups where the reverse choice has been made. The sign of z is indicated beside the "point" (small circle). In both diagrams, the $+x$ direction (a) is down the page, $+y$ (b) toward the right. A comma within the circle indicates that that point is of opposite handedness to the points without commas, as when derived from these by mirror plane or inversion operation. Where two points are related by a mirror lying in the plane of the paper, half of the circular symbol is marked with a comma, half left blank.

Below the diagrams are the lists of all possible points in this diperiodic group and equivalent point positions.

First column: Number of positions that are symmetrically equivalent, given the first position in the series.

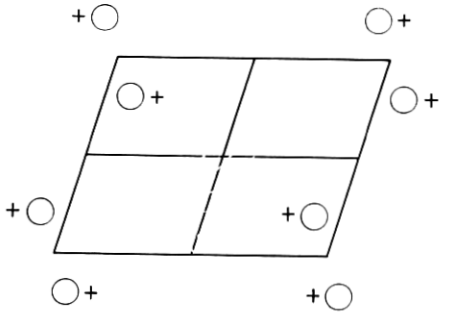
Second column: Arbitrary identifying letter, conventionally the same as that first used by Wyckoff for this position.

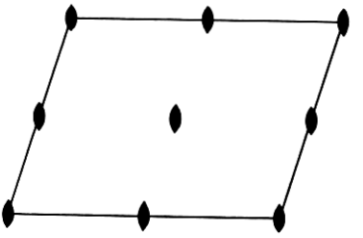
Third column: The symmetry of each point in the group (if each point lies on a two-fold axis, this will be "2"; if each point lies in a mirror plane this will be "m"; etc.). This will always be "1" for the "general position" which, by definition, is the position of a point not lying on any symmetry element.

Fourth column: Coordinates of equivalent positions. Note that not every group has "special positions." Special positions occur when a particular value of x, y, or z results in a reduction of the number of equivalent positions due to symmetry.

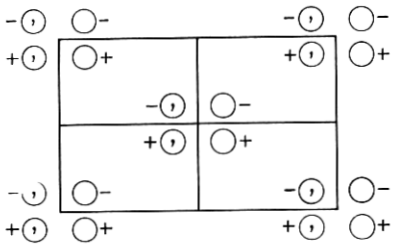
Fifth column: Conditions on hk which must be satisfied, for x-ray reflection to occur when the point positions in column 4 are occupied.

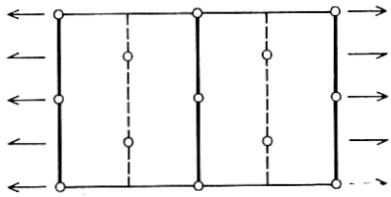
(References on page 559)



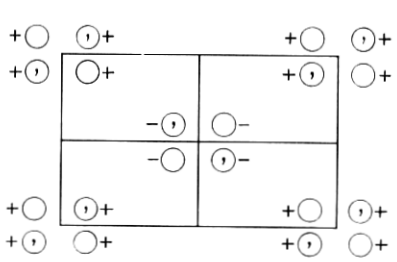


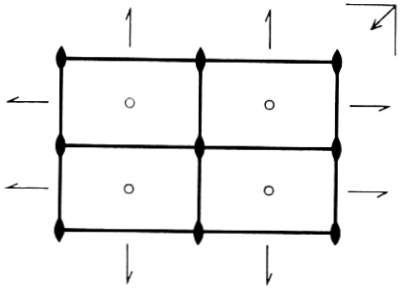
Number of positions, Wyckoff notation, and point symmetry			Co-ordinates of equivalent positions		Conditions limiting possible reflections
2	e	1	$x,y,z;$	$\bar{x},\bar{y},z.$	General: $hk:$ $h0:$ } No conditions $0k:$
1	d	2	$\frac{1}{2},\frac{1}{2},z.$		Special: No conditions
1	c	2	$\frac{1}{2},0,z.$		
1	b	2	$0,\frac{1}{2},z.$		
1	a	2	$0,0,z.$		



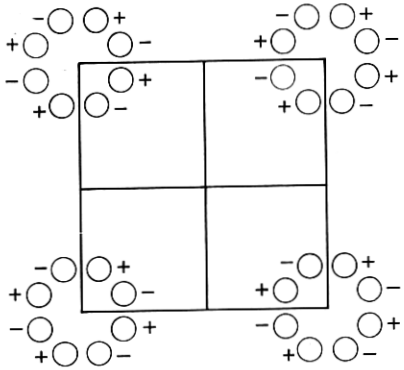


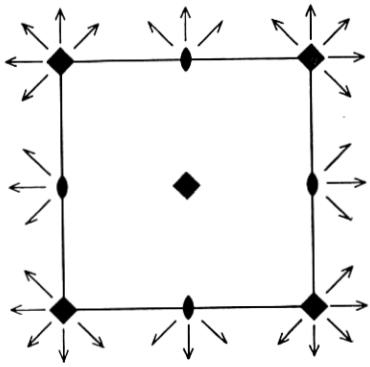
Number of positions, Wyckoff notation, and point symmetry			Co-ordinates of equivalent positions				Conditions limiting possible reflections
			$(0,0,0;\ \frac{1}{2},\frac{1}{2},0)+$				
8	j	1	$x,y,z;$	$x,\bar{y},z;$	$\bar{x},y,\bar{z};$	$\bar{x},\bar{y},\bar{z}.$	General: hk: $h+k=2n$ $h0$: $(h=2n)$ $0k$: $(k=2n)$
							Special: as above, plus
4	i	m	$x,0,z;$	$\bar{x},0,\bar{z}.$			No extra conditions
4	g	2	$0,y,0;$	$0,\bar{y},0.$			
4	e	$\bar{1}$	$\frac{1}{4},\frac{1}{4},0;$	$\frac{1}{4},\frac{3}{4},0.$			hk: $h=2n$; $(k=2n)$
2	b	$2/m$	$0,\frac{1}{2},0.$				No extra conditions
2	a	$2/m$	$0,0,0.$				



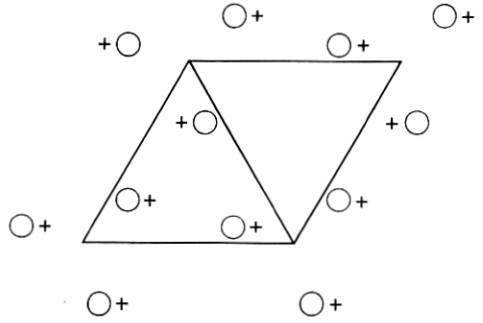


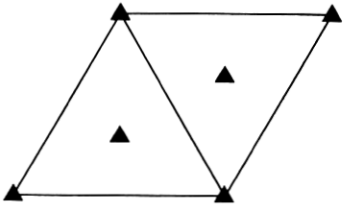
Number of positions, Wyckoff notation, and point symmetry			Co-ordinates of equivalent positions	Conditions limiting possible reflections
8	g	1	x,y,z; $\bar{x},\bar{y},z$; $\frac{1}{2}-x,\frac{1}{2}-y,\bar{z}$; $\frac{1}{2}-x,\frac{1}{2}+y,\bar{z}$; $\bar{x},y,z$; $x,\bar{y},z$; $\frac{1}{2}+x,\frac{1}{2}+y,\bar{z}$; $\frac{1}{2}+x,\frac{1}{2}-y,\bar{z}$.	General: hk: $h+k=2n$ $h0$: $(h=2n)$ $0k$: $(k=2n)$ Special: as above, plus
4	f	m	$x,0,z$; $\bar{x},0,z$; $\frac{1}{2}-x,\frac{1}{2},\bar{z}$; $\frac{1}{2}+x,\frac{1}{2},\bar{z}$.	no extra conditions
4	e	m	$0,y,z$; $0,\bar{y},z$; $\frac{1}{2},\frac{1}{2}-y,\bar{z}$; $\frac{1}{2},\frac{1}{2}+y,\bar{z}$.	no extra conditions
4	c		$\frac{1}{4},\frac{1}{4},0$; $\frac{3}{4},\frac{3}{4},0$; $\frac{1}{4},\frac{3}{4},0$; $\frac{3}{4},\frac{1}{4},0$.	hkl: $h=2n$; $k=2n$
2	b	mm	$0,\frac{1}{2},z$; $\frac{1}{2},0,\bar{z}$.	no extra conditions
2	a	mm	$0,0,z$; $\frac{1}{2},\frac{1}{2},\bar{z}$.	no extra conditions



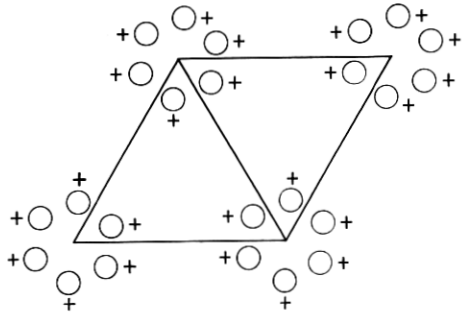


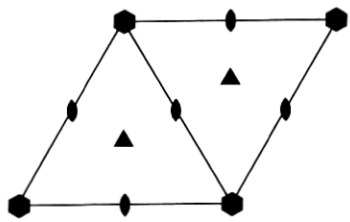
Number of positions, Wyckoff notation, and point symmetry			Co-ordinates of equivalent positions				Conditions limiting possible reflections
							General:
8	p	1	x,y,z; $\bar{y},\bar{x},\bar{z}$;	$\bar{x},\bar{y},z$; $y,x,\bar{z}$;	$\bar{x},y,\bar{z}$; $y,\bar{x},z$;	$x,\bar{y},\bar{z}$; $\bar{y},x,z$.	No conditions
							Special:
4	o	2	$x,\frac{1}{2},0$;	$\bar{x},\frac{1}{2},0$;	$\frac{1}{2},x,0$;	$\frac{1}{2},\bar{x},0$.	No conditions
4	l	2	$x,0,0$;	$\bar{x},0,0$;	$0,x,0$;	$0,\bar{x},0$.	
4	j	2	$x,x,0$;	$\bar{x},\bar{x},0$;	$\bar{x},x,0$;	$x,\bar{x},0$.	
4	i	2	$0,\frac{1}{2},z$;	$0,\frac{1}{2},\bar{z}$;	$\frac{1}{2},0,z$;	$\frac{1}{2},0,\bar{z}$.	hk: $h + k = 2n$
2	h	4	$\frac{1}{2},\frac{1}{2},z$;	$\frac{1}{2},\frac{1}{2},\bar{z}$.			No conditions
2	g	4	$0,0,z$;	$0,0,\bar{z}$.			
2	e	222	$\frac{1}{2},0,0$;	$0,\frac{1}{2},0$.			hk: $h + k = 2n$
1	c	42	$\frac{1}{2},\frac{1}{2},0$.				No conditions
1	a	42	$0,0,0$.				





Number of positions, Wyckoff notation, and point symmetry			Co-ordinates of equivalent positions	Conditions limiting possible reflections
3	d	1	$x,y,z;$ $\bar{y},x-y,z;$ $y-x,\bar{x},z.$	General: No conditions
1	c	3	$\frac{2}{3},\frac{1}{3},z.$	
1	b	3	$\frac{1}{3},\frac{2}{3},z.$	Special: No conditions
1	a	3	$0,0,z.$	





Number of positions, Wyckoff notation, and point symmetry			Co-ordinates of equivalent positions			Conditions limiting possible reflections
6	d	1	$x,y,z;$	$\bar{y},x-y,z;$	$y-x,\bar{x},z;$	General: No conditions
			$\bar{x},\bar{y},z;$	$y,y-x,z;$	$x-y,x,z.$	
3	c	2	$\frac{1}{2},0,z;$	$0,\frac{1}{2},z;$	$\frac{1}{2},\frac{1}{2},z.$	
2	b	3	$\frac{1}{3},\frac{2}{3},z;$	$\frac{2}{3},\frac{1}{3},z.$		Special: No conditions
1	a	6	$0,0,z.$			

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