LOGICAL SYMBOLS FOR POINT SYMMETRY GROUPS

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The present symbols for designating the thirty-two point symmetry groups in crystallography are needlessly complicated. These symmetry groups are so simple and logical that the fundamental symmetry elements and their relative positions can be designated completely by a newly devised set of symbols. Rather than having symbols that the student must learn and associate with the groups, the symbols can be an aid to learning the groups. The symbols which the author is proposing have so many advantages over the Schoenflies symbols that they warrant being brought to the attention of mineralogists.

With the Schoenflies symbols in order to know what groups the various symbols represent, it is necessary to learn the meaning of the principal letters, C, V, D, S, T, and O, and the subscripts or indices, i, h, v, d, s, 1, 2, 3, 4, and 6. Even after the meaning is known these letters and figures only in the simpler cases indicate the least group of symmetry operations which fully identify the class of symmetry. A logical set of symbols can be devised by recognizing that the fundamental symmetry elements are: rotation axes, rotary reflection axes, a horizontal symmetry plane, and a vertical symmetry plane, whereby the above eleven letters can be reduced to only two, the subscripts *h* and *v*.

The recognition of the rotary reflection axes in general as fundamental elements helps to bring about a considerable part of the simplification. A two-fold rotary reflection axis is equivalent to a center of symmetry; also a six-fold rotary reflection axis is equivalent to a three-fold axis, and a center of symmetry, but a four-fold rotary reflection axis in the tetragonal and cubic systems has no equivalent group of symmetry elements. Therefore, it is better to recognize all rotary reflection axes as fundamental symmetry elements.

In this new set of symbols the principal axis of the crystal is designated by a large figure such as 1, 2, 3, 4, or 6 according to the degree of symmetry of the principal axis, and in those cases where the principal axis is a rotary reflection axis, the symbols are designated by $\bar{2}$, $\bar{4}$, or $\bar{6}$. The minus sign above the figure is used to indicate that the rotary reflection axis is of a lower symmetry than that of a corresponding simple, rotation axis. Further, the subscript

2, as for example, 3_2, signifies that in addition to a three-fold principal axis the group contains a two-fold axis at right angles to the principal axis, and a subscript *h*, for example, 3_h, signifies that the group contains a horizontal plane of symmetry (that is, a plane perpendicular to the principal axis), while a subscript *v*, for example, 3_v, signifies that the group contains a vertical plane of symmetry (that is, a plane through the principal axis). If in addition to a two-fold axis at right angles to the principal axis the group contains a horizontal reflection plane, the subscript *h* is added, as for example, 3_{2h}.

These symbols have only one meaning whenever they are used; for example, 6_{2h} signifies a six-fold principal axis with both a two-fold axis and a symmetry plane at right angles to the principal axis, while $\overline{6}_2$ means a six-fold rotary reflection principal axis with a two-fold axis at right angles to it. The above described symbols indicate how the symbols for all groups can be formed, except those of the cubic system.

Those groups belonging to the cubic system have in addition to a principal axis and a two-fold axis at right angles to the principal axis, also a three-fold axis. This three-fold axis is the principal diagonal of a cube in which the principal axis passes perpendicularly through the center of the base of the cube and the two-fold axis perpendicularly through the center of the front face of the cube. For example, the lowest symmetry group in the cubic system is 2_{23}, which signifies a two-fold principal axis with a two-fold axis at right angles to it and a three-fold diagonal axis in the position with respect to these two two-fold axes as described above.

The next higher symmetry group is 2_{23h}. This designates the same set of axes as described for 2_{23}, but in addition, this group possesses a horizontal reflecting plane. Here again the subscript 3 can mean only a three-fold diagonal axis in the position described above.

Since the principal axis, the perpendicular two-fold axis, the diagonal three-fold axis, and the reflecting planes have always only the relative positions described above, the symbols for any group, therefore, not only designate the fundamental symmetry elements of the group (the least group of symmetry elements which fully identify the class of symmetry), but also their relative positions.

All the other symbols for the thirty-two point groups arranged according to crystal systems together with the corresponding

TABLE 1

Group Name		Schoenflies Symbol	New Symbol	Equivalent Points
Groth	Schoenflies			
Triclinic System				
Asymmetric pedial	Hemihedry	C_1	1	1
Pinacoidal	Holohedry	$C_i=S_2$	$\bar{2}$	2
Monoclinic System				
Domatic	Hemihedry	C_s	1_h	2
Monoclinic sphenoidal	Hemimorphic hemihedry	C_2	2	2
Monoclinic prismatic	Holohedry	C_{2h}	2_h	4
Orthorhombic System				
Rhombic pyramidal	Hemimorphic hemihedry	C_{2v}	2_v	4
Rhombic bisphenoidal	Enantiomorphic hemihedry	$V=D_2$	2_2	4
Rhombic bipyramidal	Holohedry	$V_h=D_{2h}$	2_{2h}	8
Rhombohedral System				
Trigonal pyramidal	Tetartohedry	C_3	3	3
Ditrigonal pyramidal	Hemimorphic hemihedry	C_{3v}	3_v	6
Trigonal trapezohedral	Enantiomorphic hemihedry	D_3	3_2	6
Rhombohedral	Hexagonal tetartohedry of the second sort	$C_{3i}=S_6$	$\bar{6}$	6
Ditrigonal scalenohedral	Holohedry	D_{3d}	$\bar{6}_2$	12
Tetragonal System				
Tetragonal bisphenoidal	Tetartohedry of the second sort	S_4	$\bar{4}$	4
Tetragonal scalenohedral	Hemihedry of the second sort	$V_d=D_{2d}$	$\bar{4}_2$	8
Tetragonal pyramidal	Tetartohedry	C_4	4	4
Tetragonal bipyramidal	Paramorphic hemihedry	C_{4h}	4_h	8
Ditetragonal pyramidal	Hemimorphic hemihedry	C_{4v}	4_v	8
Tetragonal trapezohedral	Enantiomorphic hemihedry	D_4	4_2	8
Ditetragonal bipyramidal	Holohedry	D_{4h}	4_{2h}	16

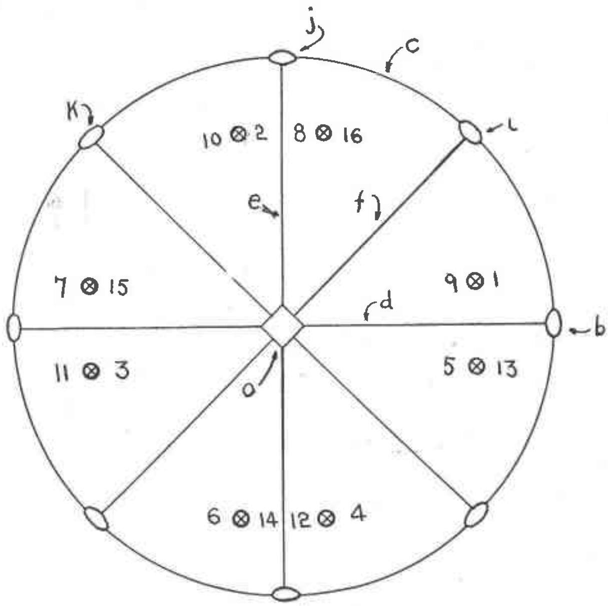
Hexagonal System

Trigonal bipyramidal	Trigonal paramorphic hemihedry	C_{3h}	3_h	6
Ditrigonal bipyramidal	Trigonal holohedry	D_{3h}	3_{2h}	12
Hexagonal pyramidal	Tetartohedry	C_6	6	6
Hexagonal bipyramidal	Paramorphic hemihedry	C_{6h}	6_h	12
Dihexagonal pyramidal	Hemimorphic hemihedry	C_{6v}	6_v	12
Hexagonal trapezohedral	Enantiomorphic hemihedry	D_6	6_2	12
Dihexagonal bipyramidal	Holohedry	D_{6h}	6_{2h}	24

Cubic System

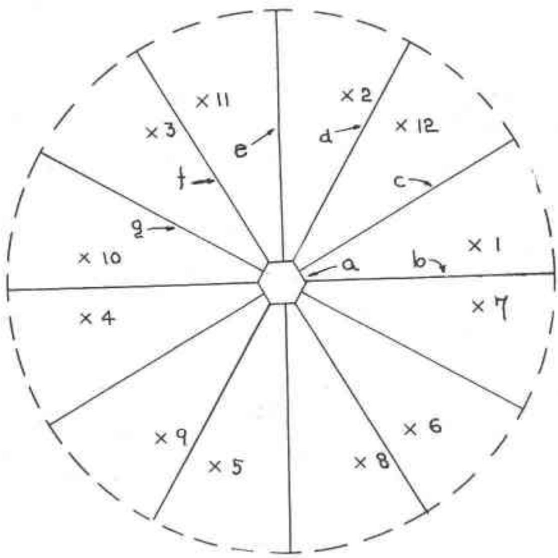
Tetrahedral pentagonal dodecahedral	Tetartohedry	T	2_{23}	12
Diacisdodecahedral	Paramorphic hemihedry	T_h	2_{23h}	24
Hexacistetrahedral	Hemimorphic hemihedry	T_d	$\bar{4}_{23}$	24
Pentagonalicositetrahedral	Enantiomorphic hemihedry	O	4_{23}	24
Hexacisoctahedral	Holohedry	O_h	4_{23h}	48

Schoenflies symbols are given in Table 1. These symbols indicate the fundamental elements of symmetry of each group. All other elements of symmetry and their relative positions can be determined from the fundamental symmetry elements as will be illustrated by constructing a stereographic projection of the equivalent points of several groups, such as groups 4_{2h}, 6_v, and $\bar{4}_{23}$. We will in each case assume the elements of symmetry and their relative positions given by the symbol and will start with one general point in the positive octant, deriving all the equivalent points by applying only the symmetry operations indicated by the symbol for that group. We will mark this first point 1 and the following points 2, 3, etc. in the order in which they are formed by the symmetry operations. The figure on the left hand side of a point is the order number of that point designated by the circle, while the right hand figure is the order number of that point designated by the cross. After all of the equivalent points of the group are found, the remaining symmetry elements can be seen at a glance from the position of the equivalent points. Figure 1 is a stereographic projection of the equivalent points of group 4_{2h}. The elements marked *a*, *b*, and *c* are the fundamental elements indicated by the symbol. Operation "*a*" gives points 2, 3, and 4. Operation "*b*" gives points 5, 6, 7, and 8. Opera-



4_{2h}

FIG. 1

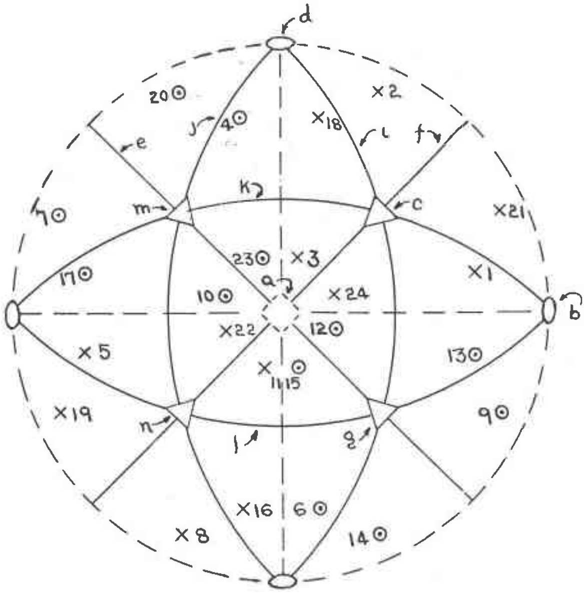


6v

FIG. 2

tion "c" gives points 9, 10, 11, 12, 13, 14, 15, and 16. From the position of the equivalent points it can be seen that the group also contains four vertical planes, d, e, f, g, and three more two-fold rotation axes, i, j, k, and a center of symmetry.

Figure 2 is group 6_v. The elements marked a and b are the fundamental elements indicated by the symbol. Operation "a" gives points 2, 3, 4, 5, and 6. Operation "b" gives points 7, 8, 9, 10, 11, and 12. From the position of the equivalent points it can be seen that the group also contains five more vertical planes, c, d, e, f, and g.



$\bar{4}_{23}$

FIG. 3

Figure 3 is group $\bar{4}_{23}$. The elements marked a, b, and c are indicated by the symbol. The element "a" is drawn in a broken line to indicate that the principal axis is a four-fold rotary reflection axis, $\bar{4}$, to distinguish it from a simple rotation axis which is indicated by the same symbol in a solid line (see Fig. 1).

In the cubic system it is easier to construct the stereographic projection of the equivalent points by first performing the three-fold rotation operation before the principal axis rotation and the other operations. Operation "*c*" gives points 2 and 3. Operation "*a*" gives points 4, 5, 6, 7, 8, 9, 10, 11, and 12, and operation "*b*" gives points 13, 14, 15, 16, 17, 18, 19, 20, 21, 22, 23, and 24. From these points it is apparent that the group also possesses another two-fold axis, *d*, and two vertical planes, *e*, and *f*, four diagonal planes, *i*, *j*, *k*, and *l*, and three more three-fold axes, *m*, *n*, and *g*.

A special feature of this new system of symbols is that the number of equivalent points in the group is indicated by the symbol itself. As a letter indicates a two-fold operation, it has an equivalent numerical value of 2. The number of equivalent points then is the product of all the figures and letters needed to constitute the symbol. In the three examples given above, the number of equivalent points is determined from the symbols as follows: From the symbol 4_{2h} we obtain (4) (2) (2) = 16 equivalent points. From the symbol 6_v we obtain (6) (2) = 12 equivalent points, while from the symbol $\bar{4}_{23}$ we obtain (4) (2) (3) = 24 equivalent points. All of these equivalent points agree with the number of equivalent points shown on Figures 1, 2, and 3. In the same way the number of equivalent points given in the last column of Table 1 can be seen to be indicated by the corresponding symbol.

These symbols can be used to designate the space groups as subdivisions of the point groups by superscripts, 1, 2, 3, etc. in exactly the same way that the space groups are designated by the Schoenflies symbols, as only subscripts are used to indicate point groups.

TABLE II

			1	1_h					
		$\bar{2}$	2	2_h	2_v	2_2	2_{2h}	2_{23}	2_{23h}
			3	3_h	3_v	3_2	3_{2h}		
$\bar{4}_{23}$	$\bar{4}_2$	$\bar{4}$	4	4_h	4_v	4_2	4_{2h}	4_{23}	4_{23h}
	$\bar{6}_2$	$\bar{6}$	6	6_h	6_v	6_2	6_{2h}		

In Table 2 the groups are rearranged to show their interrelationship. The five groups with a two-fold principal axis have corresponding groups with three-, four-, and six-fold principal axes, which form the rectangular block of twenty groups shown in the table. The other groups fit logically around this block. Since a one- or three-fold rotary reflection axis would not bring a point back to its original position after a rotation of 360° it is obvious that only two-, four-, and six-fold rotary reflection axes are possible. Combinations of a rotary reflection axis with a horizontal reflection plane do not occur, since this condition would raise the symmetry of the axis to a simple rotation axis.

In this arrangement of the groups it can be noted how with only rotation and rotary reflection axes and horizontal and vertical reflection planes all the groups build up logically from the lowest symmetry to the highest possible crystal symmetry group. This arrangement also brings out the fact that the special development to diagonal three-fold axes is possible for only those groups having a two-fold axis perpendicular to a principal axis of lower symmetry than six-fold rotary reflection. The thirty-two point groups can be remembered easily by recalling the arrangement shown in Table 2.

From Table 1 it will be noticed that all these new symbols not only designate the groups, but actually indicate the symmetry of the groups, as all the necessary symmetry elements and just those sufficient to completely classify the group are given in each symbol. These are arranged in the order of their relative importance by making the principal axis the main figure of the symbol. These symbols, therefore, actually represent the groups rather than just designate them as the Schoenflies symbols do.

Besides being more adequate the new symbols are far simpler, as only axes and planes need be designated. A figure as used in these symbols designates an axis completely, that is, the kind of axis and its relative position. This leaves only two letters necessary in these symbols to designate the planes. With only these two things to remember and with the symbol actually representing the symmetry of the group the symmetry of the group is seen at a glance from the symbol. For example in Table 1 these symbols indicate the relationship between the thirty-two symmetry groups and the seven crystal systems classification. First, all orthorhombic principal axes are two-fold, and all tetragonal principal axes are four-fold. Then, the rhombohedral system contains all the groups with three-fold principal axes, except those having horizontal reflection planes and all the groups having $\bar{6}$ principal axes, while the hexagonal system contains only those groups having three-fold axes with horizontal reflection planes, and all the groups with simple six-fold rotation axes. The distinguishing feature of the cubic system groups, the three-fold diagonal axis, is also indicated by these symbols.

The above relations are due, of course, to the fact that the holohedry group of each crystal system is the symmetry of the space lattice of that system. The crystal system classification, then, is really a symmetry group classification of the space lattices of crystals. All other lower groups in any one crystal system are produced by the interpenetration of these similar lattices which accounts, for example, for the impossibility of horizontal reflection planes in the rhombohedral system, since the rhombic space lattice has a rotary reflection principal axis, and as previously explained precludes horizontal reflection planes. All of these relations and many more are recognized directly from the symbols.

In addition to all of the advantages cited which these new symbols have over the Schoenflies symbols, over half of them are designated by fewer figures and letters than the corresponding Schoenflies symbols.

The writer has found these symbols a great help to mineralogy students in their course of "X-Ray Analysis of Crystalline Materials." Particularly were these symbols helpful in determining the space groups from the X-ray data.