

The fact that these ratios are constant means that, if these structures are oxides,  $M_3O$ , apparently only the crystal atomic diameter of the metal atoms determines the lattice constants of the  $A15$  structures mentioned. In the light of the foregoing it is remarkable that pure  $Mo_3O$ , according to Schönberg (1954*b*), does not crystallize in the  $A15$  structure.

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**The nomenclature of crystallographic symmetry groups.** By J. BOHM and K. DORNBERGER-SCHIFF, *Deutsche Akademie der Wissenschaften zu Berlin, II. Physikalisch-Technisches Institut and Institut für Strukturforschung, Berlin-Adlershof, Germany.*

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Additional to the well known crystallographic space groups and point groups there exist further kinds of symmetry group, such as groups in other than three dimensions, groups of antisymmetry, black-white symmetry, cryptosymmetry, colour symmetry, multiple symmetry and so on.

Different nomenclatures and symbols for the individual groups belonging to some of these kinds of symmetry group were proposed by various authors. But the fact that in each case these symmetry groups have geometrical representations may be used to obtain a survey and classification (Holser, 1961; Bohm, 1963), and geometrical symbols may be given to all symmetry groups. Such 'International Symbols' for the 230 space groups and the 32 point groups are familiar to crystallographers; corresponding symbols for the 80 'antisymmetric plane groups' or the 'plane space groups' have been proposed by Dornberger-Schiff (1956, 1959, 1964) and in a somewhat modified manner by Holser (1958). Geometrical symbols avoid the use of special antisymmetric or other special symmetry elements. They have the great advantage that all data given for the three-dimensional space groups in *International Tables for X-ray Crystallography* (1952) (coordinates of general and special positions, structure factor formulae *etc.*) may be used as they stand or after a simple transformation.

In this paper proposals will be made for a nomenclature of some further kinds of symmetry group. Various names of these different kinds are quoted; in this paper a symbol  $G_{rst}$ ... is used, as proposed by one of us (Bohm, 1963). In such a symbol the indices  $rst$ ... give the dimensions of the sub-spaces which remain invariant under the operations of the particular symmetry groups and lie one inside the other. (This proposal is a generalization of a proposal by Niggli 1959); details are given in Bohm (1963), where, however, no mention is made of the fact that some of the listed kinds of symmetry group are identical.)

In the following, geometrical symbols of the groups of  $G_{31}$ ,  $G_{310} = G_{320}$ ,  $G_{321}$ ,  $G_{3210}$ ,  $G_{21}$  and  $G_{210}$  are described and listed. Together with the earlier proposals (Dornberger-Schiff, 1956) they furnish a complete set of geometrical symbols for all kinds of symmetry group up to three dimensions.

#### 1. The groups of $G_{31}$ ; the groups of $G_{310}$

('Linear space groups', 'three-dimensional line groups', 'Balkengruppen', 'one-dimensional colour groups', 'one-dimensional cryptosymmetric groups', and the corresponding point groups.)

The number of the groups of  $G_{31}$  is, strictly speaking unlimited. But if only subgroups of the three-dimensional space groups are admitted, there are 75 different groups. The proposed symbols of the groups are listed in Table 1. The symbols begin with the lattice-symbol  $P$ , because the lattice of groups with a single periodicity is necessarily primitive; a capital letter is used because the objects are three-dimensional (*cf.* § 3, where  $p$  is used in  $G_{21}$  for two-dimensional objects). The symbols of the symmetry elements retain their well known meaning: 1,  $\bar{1}$ ,  $m$ ,  $c$ , 2,  $2_1$ , 3,  $\bar{3}$ ,  $3_1$ ,  $3_2$ , ... *etc.* The sequence of symbols is exactly as in space group notation; for certain cases a 1 (monad axis) is added (corresponding *e.g.* to space group  $P31m$ ). For the symmetry elements there are three positions in the symbol; the two positions corresponding to the directions of missing periodicity are put into a pair of brackets (see Table 1).

There are possibilities to write abbreviated symbols, which are not listed. Table 1 contains some further information: Those groups which permit enantiomorphy are marked by +. There exist pairs of 'enantiomorphous groups' among the  $G_{31}$  groups (as among the ordinary space groups). They contain an enantiomorphous screw axis and are not to be confused with those groups which permit enantiomorphy (*cf.* Bohm & Kleber, 1958/59). The enantiomorphous pairs are marked in Table 1 by a curly bracket before their numbers. Amongst the 75  $G_{31}$  groups there are 8 pairs of enantiomorphous groups. Symbols of the  $G_{31}$  groups according to Alexander (1929) are given in Table 1 for comparison.

The point groups  $G_{310}$  are identical with the point groups  $G_{320}$  of a 'two-sided plane' or the 'two-dimensional antisymmetric point groups'. They are listed in Table 1 side by side with the corresponding groups of  $G_{31}$ . To indicate which dimensions are transformed separately from the others the symbols of two positions are enclosed in one pair

Table 1. Symbols for the  $G_{31}$  and the  $G_{310} = G_{320}$  groups  
 The symbols for the  $G_{321}$  and  $G_{3210}$  groups are obtained as described in the text

$G_{321}$	No.	Symbol for $G_{31}$	Symbol according to		$G_{3210}$	No.	Symbol for $G_{310}$	Symbol according to	
			Alexander	Enantio-morphy				Alexander	Enantio-morphy
×	1	$P(11)1$	$C_1^0$	+	×	1	$(11)(1)$	$C_1$	+
×	2	$P(\bar{1}\bar{1})\bar{1}$	$C_i^0$		×	2	$(\bar{1}\bar{1})(\bar{1})$	$C_i$	
×	3	$P(m1)1$	$C_r^0$		×	3	$(m1)(1)$	$C_v$	
×	4	$P(c1)1$	$C_{rt}^0$						
×	5	$P(11)m$	$C_h^0$		×	4	$(11)(m)$	$C_h$	
×	6	$P(11)2$	$C_2^0$	+	×	5	$(11)(2)$	$C_2$	+
×	7	$P(11)2_1$	$C_2^1$	+					
×	8	$P(21)1$	$D_1^0$	+	×	6	$(21)(1)$	$D_1$	+
×	9	$P(11)\frac{2}{m}$	$C_{2h}^0$		×	7	$(11)\left(\frac{2}{m}\right)$	$C_{2h}$	
×	10	$P(11)\frac{2_1}{m}$	$C_{2h}^1$						
×	11	$P\left(\frac{2}{m}1\right)1$	$D_d^0$		×	8	$\left(\frac{2}{m}1\right)(1)$	$D_d$	
×	12	$P\left(\frac{2}{c}1\right)1$	$D_{dt}^0$						
×	13	$P(mm)2$	$C_{2v}^0$		×	9	$(mm)(2)$	$C_{2v}$	
×	14	$P(mc)2_1$	$C_{2v}^1$						
×	15	$P(cc)2$	$C_{2vt}^0$						
×	16	$P(2m)m$	$D_h^0$		×	10	$(2m)(m)$	$D_h$	
×	17	$P(2c)m$	$D_{ht}^0$						
×	18	$P(22)2$	$D_2^0$	+	×	11	$(22)(2)$	$D_2$	+
×	19	$P(22)2_1$	$D_2^1$	+					
×	20	$P\left(\frac{2}{m}\frac{2}{m}\right)\frac{2}{m}$	$D_{2h}^0$		×	12	$\left(\frac{2}{m}\frac{2}{m}\right)\frac{2}{m}$	$D_{2h}$	
×	21	$P\left(\frac{2}{m}\frac{2}{c}\right)\frac{2_1}{m}$	$D_{2h}^1$						
×	22	$P\left(\frac{2}{c}\frac{2}{c}\right)\frac{2}{m}$	$D_{2ht}^0$						
	23	$P3(11)$	$C_3^0$	+		13	$(3)(11)$	$C_3$	+
	24	$P3_1(11)$	$C_3^1$	+					
	25	$P3_2(11)$	$C_3^2$	+					
	26	$P\bar{3}(11)$	$C_{3i}^0$			14	$(\bar{3})(11)$	$C_{3i}$	
	27	$P3(m1)$	$C_{3v}^0$			15	$(3)(m1)$	$C_{3v}$	
	28	$P3(c1)$	$C_{3vt}^0$						
	29	$P3(21)$	$D_3^0$	+		16	$(3)(21)$	$D_3$	+
	30	$P3_1(21)$	$D_3^1$	+					
	31	$P3_2(21)$	$D_3^2$	+					
	32	$P\bar{3}(m1)$	$D_{3d}^0$			17	$(\bar{3})(m1)$	$D_{3d}$	
	33	$P\bar{3}(c1)$	$D_{3dt}^0$						
	34	$P4(11)$	$C_4^0$	+		18	$(4)(11)$	$C_4$	+
	35	$P4_1(11)$	$C_4^1$	+					
	36	$P4_3(11)$	$C_4^3$	+					
	37	$P4_2(11)$	$C_4^2$	+					
	38	$P\bar{4}(11)$	$S_4^0$			19	$(\bar{4})(11)$	$S_4$	
	39	$P4(mm)$	$C_{4v}^0$			20	$(4)(mm)$	$C_{4v}$	
	40	$P4(cc)$	$C_{4vt}^0$						
	41	$P4_2(cm)$	$C_{4v}^2$						
	42	$P4(22)$	$D_4^0$	+		21	$(4)(22)$	$D_4$	+
	43	$P4_1(22)$	$D_4^1$	+					
	44	$P4_3(22)$	$D_4^3$	+					
	45	$P4_2(22)$	$D_4^2$	+					

Table 1. (cont.)

$G_{321}$	No.	Symbol for $G_{31}$	Symbol according to Alexander	Enantio-morphy	$G_{3210}$	No.	Symbol for $G_{310}$	Symbol according to Alexander	Enantio-morphy
	46	$P\bar{4}(2m)$	$D_{2d}^0$			22	$(\bar{4})(2m)$	$D_{2d}$	
	47	$P\bar{4}(2c)$	$D_{2dt}^0$						
	48	$P\left(\frac{4}{m}\right)(11)$	$C_{4h}^0$			23	$\left(\frac{4}{m}\right)(11)$	$C_{4h}$	
	49	$P\left(\frac{4_2}{m}\right)(11)$	$C_{4h}^2$						
	50	$P\frac{4}{m}\left(\frac{2}{m}\frac{2}{m}\right)$	$D_{4h}^0$			24	$\left(\frac{4}{m}\right)\left(\frac{2}{m}\frac{2}{m}\right)$	$D_{4h}$	
	51	$P\frac{4}{m}\left(\frac{2}{c}\frac{2}{c}\right)$	$D_{4ht}^0$						
	52	$P\frac{4_2}{m}\left(\frac{2}{m}\frac{2}{c}\right)$	$D_{4h}^2$						
	53	$P6(11)$	$C_6^0$	+		25	$(6)(11)$	$C_6$	+
	54	$P6_1(11)$	$C_6^1$	+					
	55	$P6_5(11)$	$C_6^5$	+					
	56	$P6_2(11)$	$C_6^2$	+					
	57	$P6_4(11)$	$C_6^4$	+					
	58	$P6_3(11)$	$C_6^3$	+					
	59	$P\bar{3}(11)$	$C_{3h}^0$			26	$(\bar{3})(11)$	$C_{3h}$	
	60	$P6(mm)$	$C_{6v}^0$			27	$(6)(mm)$	$C_{6v}$	
	61	$P6(cc)$	$C_{6vt}^0$						
	62	$P6(mc)$	$C_{6v}^3$						
	63	$P6(22)$	$D_6^0$	+		28	$(6)(22)$	$D_6$	+
	64	$P6_1(22)$	$D_6^1$	+					
	65	$P6_5(22)$	$D_6^5$	+					
	66	$P6_2(22)$	$D_6^2$	+					
	67	$P6_4(22)$	$D_6^4$	+					
	68	$P6_3(22)$	$D_6^3$	+					
	69	$P\bar{6}(m2)$	$D_{3h}^0$			29	$(\bar{6})(m2)$	$D_{3h}$	
	70	$P\bar{6}(c2)$	$D_{3ht}^0$						
	71	$P\frac{6}{m}(11)$	$C_{6h}^0$			30	$6m(11)$	$C_{6h}$	
	72	$P\frac{6_3}{m}(11)$	$C_{6h}^3$						
	73	$P\frac{6}{m}\left(\frac{2}{m}\frac{2}{m}\right)$	$D_{6h}^0$			31	$\left(\frac{6}{m}\right)\left(\frac{2}{m}\frac{2}{m}\right)$	$D_{6h}$	
	74	$P\frac{6}{m}\left(\frac{2}{c}\frac{2}{c}\right)$	$D_{6ht}^0$						
	75	$P\frac{6_3}{m}\left(\frac{2}{m}\frac{2}{c}\right)$	$D_{6h}^3$						

of brackets, as in the corresponding  $G_{31}$  groups, and the remaining position is enclosed in another pair of brackets. In this way the symbols of the  $G_{310}$  groups may be distinguished from those of the ordinary three-dimensional point groups  $G_{30}$  (which according to our notation ought to possess three positions – if need be, filled with the monads 1 – all enclosed in one pair of brackets).

## 2. The groups of $G_{321}$ ; the groups of $G_{3210}$

(‘Double antisymmetric line groups’, ‘antisymmetric band groups’, ‘Reliefbandgruppen’, and the corresponding point groups.)

The set of the  $G_{321}$  groups is a subset of the set of the  $G_{31}$  groups (as well as of the  $G_{32}$  groups) and contains only triclinic, monoclinic and orthorhombic groups (correspond-

ing to No. 1–22 of the  $G_{31}$  groups in Table 1). The symbols for the  $G_{321}$  groups have the letter  $P$  and three positions for the symmetry elements, just like the  $G_{31}$  groups. But the two positions corresponding to the directions of missing periodicity are put into separate pairs of brackets; in this way the symbols for the  $G_{321}$  may be distinguished from those referring to the  $G_{31}$  groups. The point groups  $G_{3210}$  are treated in a similar manner. Thus e.g. the cross in column ‘ $G_{321}$ ’ of Table 1 against No. 13 means that corresponding to the symbol  $P(mm)2$  there exists a  $G_{321}$  group  $P(m)(m)2$ , and similarly, corresponding to No. 9 of the  $G_{310}$  point groups  $(mm)(2)$  there exists a  $G_{3210}$  point group  $(m)(m)(2)$ .

As mentioned above, there are among the  $G_{31}$  groups 22 triclinic, monoclinic or orthorhombic groups. But in the  $G_{321}$  groups the two axes of reference referring to the non-

Table 2. Symbols for the  $G_{21}$  and the  $G_{210}$  groups

No	Geometric representation	Black-white representation	Enantiomorphy	Symbol for $G_{21}$	No	Symbol for $G_{210}$	Leitform-symphy
1			-	$p\{1\}(1)1$	1	$[1](1)(1)$	-
2			-	$p\{2\}(1)1$	2	$[2](1)(1)$	-
3			-	$p\{1\}(1)m$	3	$[1](1)(m)$	-
4			-	$p\{1\}(m)1$	4	$[1](m)(1)$	-
5			-	$p\{1\}(g)1$			
6			-	$p\{2\}(m)m$	5	$[2](m)(m)$	
7			-				

periodic directions are not exchangeable (in contrast to the  $G_{31}$  groups). Therefore those cases in which the respective symmetry elements are different have to be counted twice. The same holds for the  $G_{3210}$  point groups. Thus 31  $G_{321}$  and 16  $G_{3210}$  groups are obtained. In Table 1 the  $G_{31}$  groups giving rise to one  $G_{321}$  group are marked by one cross, those giving rise to two different groups are marked by two crosses in the column headed  $G_{321}$ . The crosses in the column headed  $G_{3210}$  have a similar meaning. In the cases marked by two crosses the symbols originally enclosed in one pair of brackets have to be taken as they stand as well as interchanged.

### 3. The groups of $G_{21}$ ; the groups of $G_{210}$

('Band groups', 'antisymmetric line groups', and the corresponding point groups.)

A geometrical nomenclature for the  $G_{21}$  (and  $G_{210}$ ) groups may be derived in accordance with the geometrical notation of the two-dimensional space groups or plane groups  $G_2$  (or the two-dimensional point groups  $G_{20}$ , respectively). To comply with our proposal, the symbols of the principal direction of the  $G_2$  and  $G_{20}$  groups, which is given in *International Tables* in the first position of the full symbol, should be marked as referring to a direction of missing periodicity and missing extension. We suggest square brackets for this purpose. Thus e.g. the plane space groups No. 2 and No. 3 in *International Tables* (1952, 4.2) should have the symbol  $p[2]11$  and  $p[1]m1$ , respectively, and the corresponding point groups  $[2](11)$  and  $[1](m1)$ , respectively (see Table 2).

\* Another sequence might be preferable, but we do not think that this point is of great importance.

In accordance with *International Tables*\* the first position in the symbol refers to the  $z$  axis (direction perpendicular to the plane of the paper in Table 2), the second position refers to the  $x$  axis (direction downward), the last position to the  $y$  axis (direction of periodicity from left to right).

The  $G_{21}$  groups are obtained from the  $G_2$  groups by enclosing one of the unbracketed symbols in round brackets, indicating again missing periodicity, and leaving out those groups which are not compatible with this lack of periodicity. As can easily be seen, in 5 of the 7  $G_{21}$  groups the symbol enclosed in square brackets is 1. With the exception of the group  $p[2](1)1$  the square brackets may be left out altogether without ambiguity, because the letter  $p$  indicates that the groups refer to two-dimensional objects.

The symbols of the  $G_{210}$  groups are treated similarly. Both the positions referring to the directions of missing periodicity are enclosed in separate pairs of (round) brackets. Thus these symbols are distinguished from those of the  $G_{20}$  groups.

As listed in Table 2, there are 7  $G_{21}$  and 5  $G_{210}$  groups.

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