Acta Cryst. (1980). A**36**, 839–845

The Periodic System of Shubnikov Point Groups

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(*Received* 14 *January* 1980; *accepted* 21 *April* 1980)

Abstract

An arrangement of the 122 Shubnikov point groups in a periodic table is proposed, the columns of which correspond in the usual way to crystal systems. Point groups in the same row have many properties in common, including content of certain symmetry elements, analogous position in the lattice of subgroups, and compatibility with electric and magnetic effects.

1. Introduction

There are 32 ordinary crystallographic point groups and 122 crystallographic Shubnikov point groups. For shortness, we shall speak of the 122 point groups and the 32 ordinary point groups. We propose an arrangement of the 122 point groups, which we call the 'periodic table', because it turns out to have a number of analogies with the Periodic Table of chemical elements. In the case of groups, we let each period occupy a column of the table instead of a row as in the case of elements. Many properties of point groups need only be given for each row instead of each group. These properties include the subgroup relationships among all the groups belonging to the same crystal system and having space reversal, time reversal and space–time reversal among the group elements. Also, the electric and magnetic effects compatible with the point groups in a row have many properties in common, but evolve systematically as one goes from left to right in the periodic table, *i.e.* from the triclinic to the cubic system.

2. The periodic table of point groups

The periodic table of point groups is given in Table 1. Each of columns 3–8 contains the point groups belonging to one or two crystal systems, as is usually done for the 32 ordinary crystallographic point groups. Column 1 numbers the rows, column 2 gives a possible choice of the generators for the point groups in the corresponding row: N, N', $\bar{N}$, $\bar{N}'$ act along the z axis and 2, 2′, m, m' along the y axis of an orthogonal coordinate system {*i.e.* the axis of the (anti)rotation diad and the normal to the (anti)reflexion plane point in the y direction [010]}. The only exception is the cubic system, where 2, 2′, m, m' act along [110] and where N stands for 2 along [001] and 3 along [111]. Columns 3, 5 and 8 contain point groups in 16 rows. (The generators of column 2 create duplications of these in the remaining rows, as indicated between brackets.) Columns 4, 6 and 7 contain point groups in all the 31 rows, in 9 of them in two different orientations. Restricting our table to ordinary point groups and comparing with the corresponding Fig. 3.3.1 in *International Tables for X-ray Crystallography* (1952), we notice a number of differences, the most important one being the different position of $\bar{4}3m$.

Each group is identified by its short international symbol and its Schoenflies symbol. The Schoenflies symbol denotes a geometric equivalence class of point groups whereas the international symbol lends itself to expressing also the orientation of the symmetry operators by the order in which their symbols appear. We deviate from the conventions in *International Tables for X-ray Crystallography* (1952) by inverting the first and third symbols in the orthorhombic system. In terms of our orthogonal coordinate system, our conventions for symbols of symmetry operators (other than 1′) can thus be expressed as follows. In column 3 of Table 1, the symmetry operators 2, 2′, m, m' are along [010]. In columns 4–8, the first symbol denotes a symmetry operator along [001]. (Note that a slash separates the two 'first' symbols.) The second symbol denotes a symmetry operator along [010], except for the cubic system, where it is along [111]. The third symbol denotes a symmetry operator along [100] in the orthorhombic system, along $[1\sqrt{3}0]$ in the hexagonal system, and along [110] in the tetragonal and cubic systems.

The number that appears to the right of the Schoenflies symbol is the proposed number of the point group and corresponds to its first appearance as we go through the table from top to bottom and from left to right. To the right of the short international symbol appears a number distinguishing the settings, if the point group appears several times in different orientations.

The short periods have an entry exactly in those rows where the short international symbol for the

0567-7394/80/060839-07$01.00

Table 1. *The periodic system of Shubnikov point groups*

1	2	3	4	5	6	7	8
		$N = 1$	$N = 2$	$N = 3$	$N = 4$	$N = 6$	$N = [2,3]$
	Gene- rators	Triclinic	Mono- clinic	Rhombo- hedral	Tetra- gonal	Hexa- gonal	Cubic
1	N	C_1 1 1	C_2 6 2 1	C_3 29 3	C_4 45 4	C_6 76 6	T 107 23
2	$\bar{N}$	$(\bar{1})$	C_s 7 m 1	$(\bar{3})$	S_4 46 $\bar{4}$	C_{3h} 77 $\bar{6}$	$(m3)$
3	N'	$(1')$	$C_2(C_1)$ 8 $2'$ 1	$(31')$	$C_4(C_2)$ 47 $4'$	$C_6(C_3)$ 78 $6'$	$(231')$
4	$\bar{N}'$	$(\bar{1}')$	$C_s(C_1)$ 9 m' 1	$(\bar{3}')$	$S_4(C_2)$ 48 $\bar{4}'$	$C_{3h}(C_3)$ 79 $\bar{6}'$	$(m'3)$
5	$N,\bar{1}$	C_i 2 $\bar{1}$	C_{2h} 10 $2/m$ 1	C_{3i} 30 $\bar{3}$	C_{4h} 49 $4/m$	C_{6h} 80 $6/m$	T_h 108 $m3$
6	$N,1'$	$C_1 x\theta$ 3 $1'$	$C_2 x\theta$ 11 $21'$ 1	$C_3 x\theta$ 31 $31'$	$C_4 x\theta$ 50 $41'$	$C_6 x\theta$ 81 $61'$	$T x\theta$ 109 $231'$
7	$N,\bar{1}'$	$C_i(C_1)$ 4 $\bar{1}'$	$C_{2h}(C_2)$ 12 $2/m'$ 1	$C_{3i}(C_3)$ 32 $\bar{3}'$	$C_{4h}(C_4)$ 51 $4/m'$	$C_{6h}(C_6)$ 82 $6/m'$	$T_h(T)$ 110 $m'3$
8	$N',\bar{1}$	$(\bar{1}1')$	$C_{2h}(C_i)$ 13 $2'/m'$ 1	$(\bar{3}1')$	$C_{4h}(C_{2h})$ 52 $4'/m$	$C_{6h}(C_{3i})$ 83 $6'/m'$	$(m31')$
9	$\bar{N},1'$	$(\bar{1}1')$	$C_s x\theta$ 14 $m1'$ 1	$(\bar{3}1')$	$S_4 x\theta$ 53 $\bar{4}1'$	$C_{3h} x\theta$ 84 $\bar{6}1'$	$(m31')$
10	$N',\bar{1}'$	$(\bar{1}1')$	$C_{2h}(C_s)$ 15 $2'/m$ 1	$(\bar{3}1')$	$C_{4h}(S_4)$ 54 $4'/m'$	$C_{6h}(C_{3h})$ 85 $6'/m$	$(m31')$
11	$N,\bar{1},1'$	$C_i x\theta$ 5 $\bar{1}1'$	$C_{2h} x\theta$ 16 $2/m1'$ 1	$C_{3i} x\theta$ 33 $\bar{3}1'$	$C_{4h} x\theta$ 55 $4/m1'$	$C_{6h} x\theta$ 86 $6/m1'$	$T_h x\theta$ 111 $m31'$
		Mono- clinic	Ortho- rhombic				
12	$N,2$	C_2 6 2 2	D_2 17 222	D_3 34 32	D_4 56 422	D_6 87 622	O 112 432
13	N,m	C_s 7 m 2	C_{2v} 18 $2mm$ 1	C_{3v} 35 $3m$	C_{4v} 57 $4mm$	C_{6v} 88 $6mm$	T_d 113 $\bar{4}3m$
14	$N,2'$	$C_2(C_1)$ 8 $2'$ 2	$D_2(C_2)$ 19 $22'2'$ 1	$D_3(C_3)$ 36 $32'$	$D_4(C_4)$ 58 $42'2'$	$D_6(C_6)$ 89 $62'2'$	$O(T)$ 114 $4'32'$
15	N,m'	$C_s(C_1)$ 9 m' 2	$C_{2v}(C_2)$ 20 $2m'm'$ 1	$C_{3v}(C_3)$ 37 $3m'$	$C_{4v}(C_4)$ 59 $4m'm'$	$C_{6v}(C_6)$ 90 $6m'm'$	$T_d(T)$ 115 $\bar{4}'3m'$
16 *a* *b*	 $\bar{N},2$ $\bar{N},m$	$(2/m)$	C_{2v} 18 $m2m$ 2 $mm2$ 3	$(\bar{3}m)$	D_{2d} 60 $\bar{4}2m$ 1 $\bar{4}m2$ 2	D_{3h} 91 $\bar{6}2m$ 1 $\bar{6}m2$ 2	$(m3m)$
17 *a* *b*	 $N',2$ $N',2'$	$(21')$	$D_2(C_2)$ 19 $2'22'$ 2 $2'2'2$ 3	$(321')$	$D_4(D_2)$ 61 $4'22'$ 1 $4'2'2$ 2	$D_6(D_3)$ 92 $6'22'$ 1 $6'2'2$ 2	$(4321')$
18 *a* *b*	 $\bar{N}',2$ $\bar{N}',m'$	$(2/m')$	$C_{2v}(C_2)$ 20 $m'2m'$ 2 $m'm'2$ 3	$(\bar{3}'m')$	$D_{2d}(D_2)$ 62 $\bar{4}'2m'$ 1 $\bar{4}'m'2$ 2	$D_{3h}(D_3)$ 93 $\bar{6}'2m'$ 1 $\bar{6}'m'2$ 2	$(m'3m')$

Table 1 (*cont.*)

1	2	3	4	5	6	7	8
		$N=1$	$N=2$	$N=3$	$N=4$	$N=6$	$N=[2,3]$
	Gene- rators	Mono- clinic	Ortho- rhombic	Rhombo- hedral	Tetra- gonal	Hexa- gonal	Cubic
19 *a* *b*	$\bar{N}$,2' $\bar{N}$,m'	(2'/m')	$C_{2v}(C_s)$ 21 m2'm' 1 mm'2' 2	($\bar{3}$m')	$D_{2d}(S_4)$ 63 $\bar{4}$2'm' 1 $\bar{4}$m'2' 2	$D_{3h}(C_{3h})$ 94 $\bar{6}$2'm' 1 $\bar{6}$m'2' 2	(m3m')
20 *a* *b*	N',m' N',m	(m1')	$C_{2v}(C_s)$ 21 2'm'm 3 2'mm' 4	(3m1')	$C_{4v}(C_{2v})$ 64 4'm'm 1 4'mm' 2	$C_{6v}(C_{3v})$ 95 6'm'm 1 6'mm' 2	($\bar{4}$3m1')
21 *a* *b*	$\bar{N}$',m $\bar{N}$', 2'	(2'/m)	$C_{2v}(C_s)$ 21 m'm2' 5 m'2'm 6	($\bar{3}$'m)	$D_{2d}(C_{2v})$ 65 $\bar{4}$'m2' 1 $\bar{4}$'2'm 2	$D_{3h}(C_{3v})$ 96 $\bar{6}$'m2' 1 $\bar{6}$'2'm 2	(m'3m)
22	N,2,$\bar{1}$	C_{2h} 10 2/m 2	D_{2h} 22 mmm	D_{3d} 38 $\bar{3}$m	D_{4h} 66 4/mmm	D_{6h} 97 6/mmm	O_h 116 m3m
23	N,2,1'	$C_2 x\theta$ 11 21' 2	$D_2 x\theta$ 23 2221'	$D_3 x\theta$ 39 321'	$D_4 x\theta$ 67 4221'	$D_6 x\theta$ 98 6221'	$O x\theta$ 117 4321'
24	N,2,$\bar{1}$'	$C_{2h}(C_2)$ 12 2/m' 2	$D_{2h}(D_2)$ 24 m'm'm'	$D_{3d}(D_3)$ 40 $\bar{3}$'m'	$D_{4h}(D_4)$ 68 4/m'm'm'	$D_{6h}(D_6)$ 99 6/m'm'm'	$O_h(O)$ 118 m'3m'
25	N,m',$\bar{1}$	$C_{2h}(C_i)$ 13 2'/m' 2	$D_{2h}(C_{2h})$ 25 mm'm' 1	$D_{3d}(C_{3i})$ 41 $\bar{3}$m'	$D_{4h}(C_{4h})$ 69 4/mm'm'	$D_{6h}(C_{6h})$ 100 6/mm'm'	$O_h(T_h)$ 119 m3m'
26	N,m,1'	$C_s x\theta$ 14 m1' 2	$C_{2v} x\theta$ 26 2mm1' 1	$C_{3v} x\theta$ 42 3m1'	$C_{4v} x\theta$ 70 4mm1'	$C_{6v} x\theta$ 101 6mm1'	$T_d x\theta$ 120 $\bar{4}$3m1'
27	N,m$\bar{1}$'	$C_{2h}(C_s)$ 15 2'/m 2	$D_{2h}(C_{2v})$ 27 m'mm 1	$D_{3d}(C_{3v})$ 43 $\bar{3}$'m	$D_{4h}(C_{4v})$ 71 4/m'mm	$D_{6h}(C_{6v})$ 102 6/m'mm	$O_h(T_d)$ 121 m'3m
28 *a* *b*	N'm, $\bar{1}$ N',m',$\bar{1}$	(2/m1')	$D_{2h}(C_{2h})$ 25 m'mm' 2 m'm'm 3	($\bar{3}$m1')	$D_{4h}(D_{2h})$ 72 4'/mmm' 1 4'/mm'm 2	$D_{6h}(D_{3d})$ 103 6'/m'mm' 1 6'/m'm'm 2	(m3m1')
29 *a* *b*	$\bar{N}$,2,1' $\bar{N}$,m,1'	(2/m1')	$C_{2v} x\theta$ 26 m2m1' 2 mm21' 3	($\bar{3}$m1')	$D_{2d} x\theta$ 73 $\bar{4}$2m1' 1 $\bar{4}$m21' 2	$D_{3h} x\theta$ 104 $\bar{6}$2m1' 1 $\bar{6}$m21' 2	(m3m1')
30 *a* *b*	N',m',$\bar{1}$' N',m,$\bar{1}$'	(2/m1')	$D_{2h}(C_{2v})$ 27 mm'm 2 mmm' 3	($\bar{3}$m1')	$D_{4h}(D_{2d})$ 74 4'/m'm'm 1 4'/m'mm' 2	$D_{6h}(D_{3h})$ 105 6'/mm'm 1 6'/mmm' 2	(m3m1')
31	N,2,$\bar{1}$,1'	$C_{2h} x\theta$ 16 2/m1' 2	$D_{2h} x\theta$ 28 mmm1'	$D_{3d} x\theta$ 44 $\bar{3}$m1'	$D_{4h} x\theta$ 75 4/mmm1'	$D_{6h} x\theta$ 106 6/mmm1'	$O_h x\theta$ 122 m3m1'

Table 2. *The abstract groups corresponding to the point groups in Table* 1

Rows	Group order	$n=1$	$n=2$	$n=3$	$n=4$	$n=6$	$n=12$
		Triclinic	Monoclinic	Rhombohedral	Tetragonal	Hexagonal	Cubic
1–4 5–10 11	n $2n$ $4n$	C_1 C_2 D_2	C_2 D_2 D_{2h}	C_3 C_6 C_{6h}	C_4 C_{4h} $C_{4h} x\theta$	C_6 C_{6h} $C_{6h} x\theta$	T T_h $T_h x\theta$
		Monoclinic	Orthorhombic				
12–21 22–30 31	$2n$ $4n$ $8n$	C_2 D_2 D_{2h}	D_2 D_{2h} $D_{2h} x\theta$	D_3 D_6 D_{6h}	D_4 D_{4h} $D_{4h} x\theta$	D_6 D_{6h} $D_{6h} x\theta$	O O_h $O_h x\theta$

tetragonal and hexagonal groups begin with a 4 or 6 respectively, *i.e.* where the group contains a rotation tetrad or hexad.

The monoclinic point groups appear twice in the same order, once in column 3 and once in column 4. The nine tetragonal and nine hexagonal groups with different entries in the second and third position appear twice. The six orthorhombic point groups with two different entries in positions 1–3 appear three times, the one with three different entries appears six times. Except for the monoclinic system the multiple entries appear because those point groups are contained in the corresponding holohedry in several different orientations.

The generators determine which point groups appear in the same row and which ones in the same column. But how did we choose the order of the rows and columns? The number of elements in the point groups in rows 1–4 is n, in rows 5–10 and 12–21 $2n$, in rows 11 and 22–30 $4n$, and in row 31 $8n$, where $n = 1$, 2, 3, 4, 6 and 12 for columns 3–8. This shows that the requirement that the order of the point groups should increase from left to right has determined the arrangement of the columns uniquely. The rows have been arranged according to increasing order of the point groups as far as this is possible without mixing triclinic and monoclinic, monoclinic and orthorhombic groups in columns 3 and 4 of Table 1. Within each column the point groups in rows 1–4 are isomorphic as are those in rows 5–10, 12–21, 22–30. Table 2 gives the abstract groups that correspond to the point groups (*cf.* Ascher & Janner, 1965). The order of isomorphic rows has been chosen such that the arrangement of generator sets in column 2 of Table 1 shows a maximum of regularities. These regularities will in many cases become more visible if we write instead of our choice of generators, which was made to resemble the international symbol, a number of possible choices, *e.g.* for rows 8–10 $(N', \bar{1}) = (\bar{N}', \bar{1})$, $(\bar{N}', 1') = (\bar{N}, 1')$, $(\bar{N}, \bar{1}') = (N', \bar{1}')$.

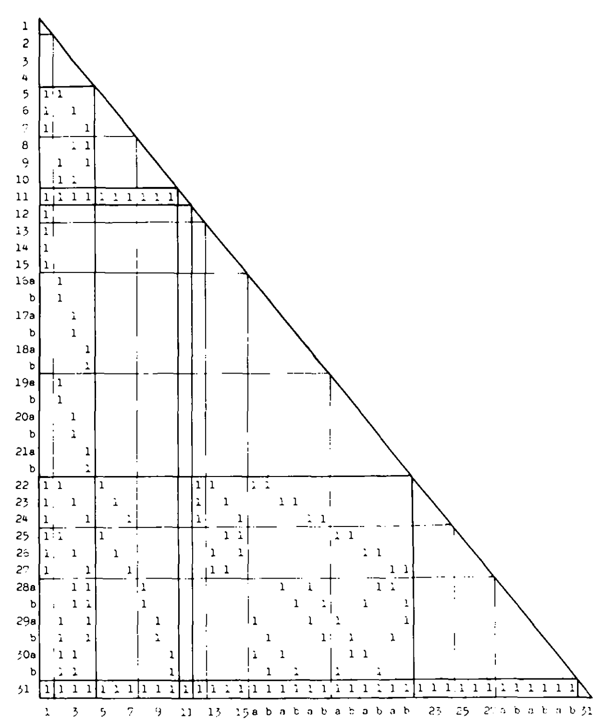
3. The subgroup relationships within each column of the periodic table

Ascher & Janner (1965) determined all the subgroups of the Shubnikov point groups, counting the subgroups as often as they appear in different orientations in the group under consideration. They presented their results in the form of a 122 × 122 triangular matrix. We shall consider the subgroup relationships only within each column of our periodic table, but we shall distinguish geometrically equivalent point groups in different orientations, which has the consequence that the elements of our matrix are either 0 or 1. We found that the same matrix (Table 3) describes the subgroup relationships within each of the long periods. Crossing out its rows and columns that correspond to rows of the periodic table without entry in the short periods, the resulting matrix describes the subgroup relationships within each of the short periods.

We find, for example, the hexagonal subgroups of a hexagonal point group if we let the numbers of rows and columns in Table 3 refer to the point groups in column 7 of Table 1. Row 25 in the matrix tells us then that $6/mm'm'$ contains the hexagonal subgroups 6, $\bar{6}$, $6/m$, $62'2'$, $6m'm'$, $\bar{6}2'm'$, and $\bar{6}m'2'$. The columns give the supergroups: column 21 b, for example, tells us in the tetragonal interpretation that $\bar{4}'2'm$ is contained in $4/m'mm$, $4'/mm'm$, $\bar{4}2m1'$ and $4/mmm1'$.

Another description of the subgroup relationship among the point groups in a column of the periodic table is given in Fig. 1. The numbers refer to the rows of Table 1. Fig. 1 admits four interpretations according to which of the four lines we read in the boxes. Reading the top line, we obtain the subgroup relationship in the short periods; the four interpretations together give the subgroup relationship in the long periods. Fig. 1 is equivalent to Table 3; in fact we can reconstruct Table 3 as follows: the matrix element in row m and column n is 1 if and only if (a) m and n stand in their boxes on the same line and (b) the box containing n can be reached from the one containing m by going downwards along a marked path. Fig. 1 also shows that Table 3 could have

Table 3. *The subgroups of the Shubnikov point groups that appear in the same column of the periodic system*



been replaced by a 16 × 16 triangular matrix with four sets of numbering for its rows and columns.

Only a small amount of information is needed in addition to Fig. 1 to write down all the subgroup relationships among the 3 × 40 + 3 × 16 = 168 *oriented* point groups; *i.e.* to derive the corresponding 168 × 168 triangular matrix. Obviously, it suffices to give the maximal subgroups that appear in other columns of Table 1. The groups in columns 8 and 7 of Table 1 have two such maximal subgroups, those in columns 6, 5, 4 one, and those in column 3 none. Examples: this maximal subgroup of the monoclinic–orthorhombic and rhombohedral groups is the triclinic–monoclinic group in the same box of Fig. 1; one of those two maximal subgroups of the hexagonal groups is the rhombohedral group in the same box of Fig. 1.

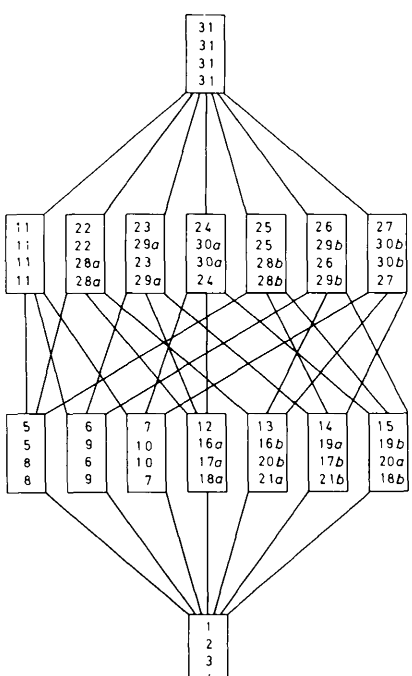


Fig. 1. The lattice of subgroups of the Shubnikov point groups in a column of the periodic table. The numbers refer to the rows of Table 1. The four rows in the boxes correspond to the four possible interpretations of the figure: the top row gives the subgroup relationship for the short periods, the four interpretations together the subgroup relationship for the long periods.

4. On electric and magnetic effects compatible with the point-group symmetry

Table 4 is a periodic table with additional information on properties shared by the point groups in each row. This time we wrote instead of the Schoenflies symbol the short international symbol that is conventionally chosen if one does not want to specify the orientation of the point group. Point groups appearing more than once (*i.e.* the monoclinic and certain orthorhombic groups) possess all the attributes listed in columns 2–4 in the rows in which the point group appears. As an example, $m'm2'$, which appears in rows 19, 20 and 21, has the attributes H, E, EH, HEE, EHH, M, P, V, s, t, u.

Column 4 indicates whether the groups in the corresponding row contain space inversion S, time inversion T, or space–time inversion U. s, t, u indicate that the group contains the corresponding inversions only in combination with a rotation.

The rows marked with an M in column 3 contain a total of 31 different non-cubic point groups. The point-group symmetry of a ferro- or ferri-magnetic domain must be one of these point groups. Similarly, the 31 different non-cubic point groups in the rows marked with a P are the possible point groups of ferro- and ferri-electric domains. A crystal with one of the 31 different non-cubic point groups contained in the rows marked with a V leaves non-vanishing velocities in certain directions invariant (*cf.*, for example, Ascher, 1974; Schmid, 1973). Triclinic point groups marked with an M, P or V are compatible with a permanent spontaneous magnetization, polarization, or current density in any direction; for monoclinic point groups these quantities may in some cases lie in a plane, in others they are restricted to a fixed direction; for orthorhombic, rhombohedral, tetragonal and hexagonal point groups these quantities are always restricted to a single direction, and for cubic point groups they must vanish altogether (Ascher & Janner, undated).

Crystals with non-cubic point groups with the attribute M are pyro-, ferro-* or ferri-magnetic; crystals with a point group containing time inversion T will be diamagnetic, paramagnetic or antiferromagnetic; the remaining crystals are antiferromagnetic. Analogously, crystals with non-cubic point groups with the attribute P are pyro-, ferro-* or ferri-electric; crystals with a point group containing space inversion S are ortho-electric, paraelectric or antiferroelectric; the remaining crystals are antiferroelectric (*cf.* Table II of Schmid, 1973).

Let g denote the density of stored free enthalpy. Its Taylor expansion with respect to the electric field E and the magnetic field H may, among others, contain the following terms

$$-g = \chi_i^0 H_i + \kappa_i^0 E_i + \alpha_{ik} E_i H_k + \tfrac{1}{2}\alpha_{ijk} H_i E_j E_k + \tfrac{1}{2}\beta_{ijk} E_i H_j H_k.$$

χ_i^0 is the spontaneous magnetization, κ_i^0 the spontaneous polarization, α_{ik} the magnetoelectric

* If the point group lies in one of columns 5 or 6 of Table 4 (*i.e.* if it belongs to the triclinic, monoclinic or orthorhombic system), weak ferromagnetism or weak ferroelectricity respectively is also possible.

Table 4. *The periodicity of the electric and magnetic effects compatible with the point groups*

1	2	3	4	Triclinic	Monoclinic	Rhombohedral	Tetragonal	Hexagonal	Cubic
1	(*H*) (*E*) *EH* *HEE* *EHH*	*MPV*		1	2	3	4	6	23
2	*H* (*EH*) *HEE* *EHH*	*M*	*s*		*m*	$\bar{4}$		$\bar{6}$	
3	*E* (*EH*) *HEE* *EHH*	*P*	*t*		2'		4'	6'	
4	*EH* *HEE* *EHH*	*V*	*u*		*m'*		$\bar{4}'$	$\bar{6}'$	
5	(*H*) *HEE*	*M*	*S*	$\bar{1}$	2/*m*	$\bar{3}$	4/*m*	6/*m*	*m*3
6	(*E*) *EHH*	*P*	*T*	1'	21'	31'	41'	61'	231'
7	*EH*	*V*	*U*	$\bar{1}'$	2/*m'*	$\bar{3}'$	4/*m'*	6/*m'*	*m'*3
8	*HEE*		*Stu*		2'/*m'*		4'/*m*	6'/*m'*	
9	*EHH*		*sTu*		*m*1'		$\bar{4}1'$	$\bar{6}1'$	
10	(*EH*)		*stU*		2'/*m*		4'/*m'*	6'/*m*	
11			*STU*	$\bar{1}1'$	2/*m*1'	$\bar{3}1'$	4/*m*1'	6/*m*1'	*m*31'
				Monoclinic	Orthorhombic				
12	*EH* (*HEE*) (*EHH*)			2	222	32	422	622	432
13	(*E*) (*EH*) (*HEE*) *EHH*	*PV*	*s*	*m*	*mm*2	3*m*	4*mm*	6*mm*	$\bar{4}3m'$
14	(*H*) (*EH*) *HEE* (*EHH*)	*M V*	*t*	2'	22'2'	32'	42'2'	62'2'	4'32'
15	(*H*) (*E*) *EH* *HEE* *EHH*	*MP*	*u*	*m'*	*m'm'*2	3*m'*	4*m'm'*	6*m'm'*	$\bar{4}'3m'$
16	(*EH*) *HEE* *EHH*		*s*		*mm*2		$\bar{4}2m$	$\bar{6}m2$	
17	(*EH*) *HEE* *EHH*		*t*		22'2'		4'22'	6'22'	
18	*EH* *HEE* *EHH*		*u*		*m'm'*2		$\bar{4}'2m'$	$\bar{6}'m'2$	
19	*H* (*EH*) *HEE* *EHH*	*M*	*stu*		*m'm*2'		$\bar{4}2'm'$	$\bar{6}m'2'$	
20	*E* (*EH*) *HEE* *EHH*	*P*	*stu*		*m'm*2'		4'*mm'*	6'*mm'*	
21	*EH* *HEE* *EHH*	*V*	*stu*		*m'm*2'		$\bar{4}'2'm$	$\bar{6}'m2'$	
22	(*HEE*)		*S*	2/*m*	*mmm*	$\bar{3}m$	4/*mmm*	6/*mmm*	*m*3*m*
23	(*EHH*)		*T*	21'	2221'	321'	4221'	6221'	4321'
24	*EH*		*U*	2/*m'*	*m'm'm'*	$\bar{3}'m'$	4/*m'm'm'*	6/*m'm'm'*	*m'*3*m'*
25	(*H*) *HEE*	*M*	*Stu*	2'/*m'*	*m'm'm*	$\bar{3}m'$	4/*mm'm'*	6/*mm'm'*	*m*3*m'*
26	(*E*) *EHH*	*P*	*sTu*	*m*1'	*mm*21'	3*m*1'	4*mm*1'	6*mm*1'	$\bar{4}3m1'$
27	(*EH*)	*V*	*stU*	2'/*m*	*mmm'*	$\bar{3}'m$	4/*m'mm*	6/*m'mm*	*m'*3*m*
28	*HEE*		*Stu*		*m'm'm*		4'/*mmm'*	6'/*m'mm'*	
29	*EHH*		*sTu*		*mm*21'		$\bar{4}2m1'$	$\bar{6}m21'$	
30	(*EH*)		*stU*		*mmm'*		4'/*m'm'm*	6'/*mmm'*	
31			*STU*	2/*m*1'	*mmm*1'	$\bar{3}m1'$	4/*mmm*1'	6/*mmm*1'	*m*3*m*1'

susceptibility, and α_{ijk}, β_{ijk} are non-linear magnetoelectric susceptibilities. Column 2 of Table 4 states which terms in the above expression need not vanish because of the point-group symmetry. A quantity between brackets means that the corresponding term is permitted by all point groups in the row except the rightmost (cubic or hexagonal) one. If the quantity is not between brackets, the term is permitted by each point group in the row. The linear magnetoelectric effect is permitted in the 58 point groups with the attribute *EH*. Apart from certain hexagonal and cubic point groups, all the point groups that contain neither space inversion *S* nor time inversion *T* do possess the attribute *EH*. Analogously, with the exception of certain hexagonal and cubic point groups, the kinetoelectric effect is permitted in all the point groups that contain neither *T* nor *U* and the kinetomagnetic effect in those that contain neither *S* nor *U*. In total there are 58 different point groups permitting the magnetoelectric effect, 58 permitting the kinetoelectric effect, and 58 permitting the kinetomagnetic effect (Ascher, 1974). The 66 different point groups with the attribute *HEE* and the 66 different point groups with the attribute *EHH* permit the second-order magnetoelectric effects I and II respectively. Those with *EHH* permit also piezoelectricity and the linear electro-optic (Pockels) effect, those with *HEE* piezomagnetism and the linear magneto-optic ('Mockels') effect. These and further effects permitted by *EHH* and *HEE* are listed in Table I of Schmid (1973).

The purpose of this paper is not to describe the above-mentioned effects but just to show that our periodic system of point groups places those groups together that are compatible with a given effect.

5. Discussion

We note analogies between the periodic tables of elements and of point groups. In both cases there are a little over a 100 items arranged in periods of different lengths. As some elements with low atomic number, especially hydrogen, have properties that do not allow us to associate them uniquely with one column, some of the point groups with low number have properties that require repeating them in different rows. The chemical elements in a column of the periodic system have properties that remain the same in the whole column, *e.g.* the number of valence electrons, and others that evolve along the column, *e.g.* the boiling point. Similarly, we found properties that remained the same in a row, *e.g.* the subgroup structure, and others that evolved along a row, *e.g.* the number of dimensions in which spontaneous magnetization or polarization is permitted.

It is a pleasure to thank Professor H. Wondratschek for his suggestions, which led to substantial improvements of the present paper.

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Acta Cryst. (1980). A**36**, 845–850

A Simple Characterization of the Subgroups of Space Groups*

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(*Received* 10 *January* 1980; *accepted* 8 *May* 1980)

Abstract

The subgroups of finite index of any n-dimensional space group are determined by the solutions of a set of congruences analogous in form and meaning to the Frobenius congruences which characterize the space groups themselves. These congruences can be solved in any dimension in which the space groups are known.

Introduction

The subgroups of the space groups play a central role both in theoretical crystallography and in the interpretation of experiment. For this reason, they have been studied intensively since Hermann first discussed them fifty years ago (Hermann, 1929). Hermann singled out two classes of subgroups for special attention, those which have the same translation subgroup as the original group (translation-equivalent subgroups) and those which belong to the same geometric crystal class as the original group (class-equivalent subgroups). This is justified by Hermann's well-known theorem that *any* subgroup is a class-equivalent subgroup of a translation-equivalent subgroup.

Following Hermann, attention has been focused on finding sequences of maximal subgroups. Recently, however, it has been shown that several contemporary problems require instead a direct knowledge of the subgroups of a given (finite) index. Thus Billiet (1977, 1978) has pointed out the usefulness of a direct approach for understanding phase transitions, and this has also been shown to be effective in the theory of color symmetry, in which the k-color groups associated with a given space group are determined by its subgroups of index k (van der Waerden & Burckhardt, 1961; Senechal, 1979).

In this paper we present a simple method for finding all the subgroups of any finite index of any n-dimensional space group. It is well known (Zassenhaus, 1948; Burckhardt, 1966) that the space groups themselves are determined by the vector solutions of a set of lattice congruences called Frobenius congruences or characteristic congruences. We show that their subgroups are also determined by a set of congruences, which are completely analogous to the Frobenius congruences in form and in meaning. Thus, in principle, the subgroups can be determined in a simple way. The congruences can be solved in any dimension in which the space groups themselves are known. And since the solutions of the 'Frobenius subgroup congruences' are vectors with integer coordinates, in many cases they can quickly be found 'by hand' using the theory of linear congruences of elementary number theory.

For brevity it is assumed that the reader is familiar with elementary number theory, linear algebra and group theory, and with the space groups in two and three dimensions.

* This paper is based on work carried out at the Institute of Crystallography, Moscow, under the auspices of the exchange program between the Academy of Sciences of the USSR and the National Academy of Sciences of the USA. It was presented to the Symposium on Mathematical Crystallography, Riederalp, Switzerland, in August 1979, held in honor of Professor Werner Nowacki.

0567-7394/80/060845-06$01.00