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On Maximal Subgroups with Increased Unit Cells

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According to Hermann [*Z. Kristallogr.* (1929), **69**, 533] the crystallographic space groups *G* have two kinds of maximal subgroups *H*, isotranslational ('zellengleich') and isoclass ('klassengleich'), *i.e.* subgroups of the same class but with different translation lattices. The maximal subgroups of index two are easily found from the existing tabulations of magnetic space groups. The paper focuses mainly on isoclass subgroups with increased unit cells. Also, a method is described for deriving directly from the crystallographic space groups all maximal isoclass subgroups of index two and of index four with increased unit cells.

Introduction

Hermann (1929) was first to distinguish between two categories of maximal subgroups *H* of space groups *G*: (*a*) subgroups *H* having the same translation lattice as *G* ('zellengleich'), (*b*) subgroups *H* having a different translation lattice, but belonging to the same crystal class as *G* ('klassengleich').

Subgroups of category (*a*) were first presented by Hermann in *Internationale Tabellen zur Bestimmung von Kristallstrukturen* (1935), so many crystallographers will be familiar with them. Subgroups of category (*b*) look more mysterious. It might even be surprising to learn from this paper that maximal subgroups of category (*b*) were first tabulated nearly 20 years ago although in a form in which the fact is difficult to recognize. Indeed, we shall show in Part I that, with little calculation, maximal subgroups of category (*b*) can be read directly from the known tabulation of magnetic space groups having an antitranslation element (Opechowski & Guccione, 1965; Belov, Neronova & Smirnova, 1957; abbreviated OG and B respectively).

In Part II, we state the rules for deriving maximal subgroups of category (*b*) directly from the crystallographic space groups. The subgroups considered are of index two and four.

Part I

I. 1. *Definitions*

Two cases are to be considered under category (*b*): (*b*1) the subgroup *H* has an increased unit cell; this case mainly will be considered here [for completeness the other cases, (*a*) and (*b*2) are dealt with in the last remarks of § I. 4.], (*b*2) the space group *G* is centred while *H* has partly or wholly lost the centring, the case for which the unit cells remain the same. In this respect the wording 'zellengleich' for category (*a*) is not particularly satisfactory. We would recommend the terminology 'isotranslation' and 'isoclass' subgroups for 'zellengleich' and 'klassengleich' respectively.

Let *G* be a group, *H* a subgroup of *G*, *g* an element of *G*, but not contained in *H*. If

$$G = H + gH\,, \qquad (1.\,1)$$

H is a maximal subgroup of index two of *G*.

(*a*) If *G* is a space group and $g=(\alpha|\tau_\alpha)$, a space group element, where α is a rotation, τ_α a translation, then *H* is a subgroup of category (*a*).

(*b*) If *G* is a space group and $g=(e|\mathbf{t}_G)$ where *e* is the identity element and $\mathbf{t}_G$ a (non-zero) lattice translation, not contained in *H*, then *H* is a subgroup of category (*b*).

I. 2. *Digression on magnetic groups*

A magnetic space group G_m is isomorphous with a space group G. We can always construct a magnetic space group from (1. 1) by the formula (Opechowski & Guccione, 1965):

$$G_m = EH + E'gH = H + g'H \,. \qquad (1.\,2)$$

Here E and E' are elements of the time-reversal group, $g' = E'g$ is an antisymmetry element. H contains all the symmetry elements, $g'H$ all the antisymmetry elements of G_m. Thus G and G_m have a common maximal subgroup H.

If $g = (\alpha|\tau_\alpha)$, the translation lattices of G_m and H and therefore the magnetic and crystallographic translation lattices (and unit cells) will be identical.

If g' is an antitranslation, the translation lattices of H will be different from those of G. Thus our task is reduced to reading from the existing tabulations of G_m first the associated (isomorphous) space group G and second the maximal subgroup H.

I. 3. *Translation groups*

We consider first the simplest case where G coincides with its translation group T. Let T be the translation group formed by all translations $\mathbf{R}_l$

$$\mathbf{R}_l = l_1\mathbf{a}_1 + l_2\mathbf{a}_2 + l_3\mathbf{a}_3 \quad (l_j \text{ integer}) \qquad (1.\,3)$$

and select all those translations for which l_3 is even, say

$$l_3 = 2l'_3 \,.$$

These translations form a group of translations T_{2a_3} in which the unit cell is $a_1, a_2, 2a_3$. We can write

$$T = T_{2a_3} + (e|\mathbf{a}_3)T_{2a_3} \,. \qquad (1.\,4)$$

Magnetic translation groups. Consider the 'wavevector'

$$\mathbf{k} = [00\tfrac{1}{2}] = \tfrac{1}{2}\mathbf{a}_3^* \qquad (1.\,5)$$

where the asterisk means 'reciprocal lattice vector'. One finds for the character of R_l

$$\chi(\mathbf{R}_l) = \exp(2\pi i \mathbf{k} \,.\, \mathbf{R}_l) \qquad (1.\,6a)$$

$$= \exp \pi i l_3 \begin{cases} = +1 \text{ for } l_3 = \text{even} \\ = -1 \text{ for } l_3 = \text{odd} \,. \end{cases} \qquad (1.\,6b)$$

Thus we have constructed a magnetic lattice T_m, *i.e.* we have partitioned the lattice of T into two parts, translations with $\chi(\mathbf{R}_l) = 1$ and 'antitranslations' with $\chi(\mathbf{R}_l) = -1$. Consequently we can write the group T_m isomorphous with T (1. 4):

$$T_m = T_{2a_3} + (e|\mathbf{a}_3)'T_{2a_3} \qquad (1.\,4')$$

where $(e|\mathbf{a}_3)'$ is an antitranslation. The present example expresses the well known fact that halving in reciprocal space (1. 5) corresponds to doubling in direct space. Actually the author previously has shown that all magnetic translation lattices can be described by invariant $\mathbf{k}$ vectors (Bertaut, 1975*a*), having components equal to 0, $\frac{1}{2}$ and 1 only. We are here more particularly interested in those $\mathbf{k}$ vectors for which at least one component is $\frac{1}{2}$. They are given in Table 1 for the magnetic translation lattices with the corresponding OG and B notation.

OG notation: the first letter, a capital, is the symbol of the lattice type to which the 'chemical' cell a_1, a_2, a_3 belongs. The subscript indicates the new periodicity of the increased unit cell.

B notation: the first letter, a capital, is the symbol of the lattice type to which the multiple cell belongs. The subscript indicates the antitranslation. We retain from these notations that, suppressing the subscripts, the OG notation indicates the lattice type of unit cell a_1, a_2, a_3 while the B notation contains the lattice type of the subgroup with the increased unit cell. More generally, consider the coset decomposition of the translation lattice T

$$T = T_0 + (e|\mathbf{t})T_0 \,. \qquad (1.\,7)$$

If $\mathbf{t}$ is a non-fractional translation, T_0 is associated with the increased unit-cell dimension $2\mathbf{t}$ (category *b*1). If T is a centred group and $\mathbf{t}$ a centring translation, T_0 is associated with the same unit cell as T, but having lost the centring $\mathbf{t}$ (category *b*2). The same reasoning as above applies to these lattices, which for completeness are summarized in Table 2 with their OG and B notation and the corresponding $\mathbf{k}$ vectors.

We now return to multiple cells. In this discussion we distinguish two cases.

Case 1. *The unit cell $a_1a_2a_3$ belongs to a P lattice*

$\mathbf{k} = [\frac{1}{2}00]$. This case has been already discussed above. The translation subgroup of lattice $2a_1, a_2, a_3$ is also of type P (B notation). The same is true for $\mathbf{k} = [0\frac{1}{2}0]$ and $\mathbf{k} = [00\frac{1}{2}]$.

Table 1. *Magnetic translation lattices with multiple cells and wavevectors* $\mathbf{k}$

OG is Opechowski–Guccione, B is Belov notation.

System	Lattice OG	Lattice B	Vector $\mathbf{k}$	System	Lattice OG	Lattice B	Vector $\mathbf{k}$
Triclinic	P_{2s}	P_s	$00\frac{1}{2}$	Orthorhombic	C_{2c}	C_c	$00\frac{1}{2}$
Monoclinic	P_{2a}	P_a	$\frac{1}{2}00$		C_I	I_c	$10\frac{1}{2}$
	P_{2b}	P_b	$0\frac{1}{2}0$	Tetragonal	P_{2c}	P_c	$00\frac{1}{2}$
	P_C	C_a	$\frac{1}{2}\frac{1}{2}0$		P_P	P_C	$\frac{1}{2}\frac{1}{2}0$
	C_{2c}	C_c	$00\frac{1}{2}$		P_I	I_c	$\frac{1}{2}\frac{1}{2}\frac{1}{2}$
Orthorhombic	P_{2a}	P_a	$\frac{1}{2}00$	Rhombohedral	R_R	R_I	$\frac{1}{2}\frac{1}{2}\frac{1}{2}$
	P_C	C_a	$\frac{1}{2}\frac{1}{2}0$	Hexagonal and trigonal	P_{2c}	P_c	$00\frac{1}{2}$
	P_F	F_s	$\frac{1}{2}\frac{1}{2}\frac{1}{2}$	Cubic	P_F	F_s	$\frac{1}{2}\frac{1}{2}\frac{1}{2}$

Table 2. *Centred translation lattices conserving the unit-cell parameters*

System	Lattice OG	Lattice B	Vector **k**
Monoclinic and orthorhombic	C_P	P_C	100
Orthorhombic	F_C	C_a	001
Orthorhombic, tetragonal and cubic	I_P	P_I	001

$\mathbf{k}=[\frac{1}{2}\frac{1}{2}0]$. In the orthorhombic and monoclinic cases, relation (1. 6*a*) shows that not only $2\mathbf{a}_1, 2\mathbf{a}_2$, but also $\mathbf{a}_1+\mathbf{a}_2$ are translations with positive character. Thus the new unit cell $2a_1, 2a_2, a_3$ is centred, *C* in the B notation.

In the tetragonal case, one does not generally conserve the increased *C* cell, but chooses the simpler tetragonal *P* cell with the translations

$$\mathbf{A}_1=\mathbf{a}_1+\mathbf{a}_2;\quad \mathbf{A}_2=\mathbf{a}_1-\mathbf{a}_2;\quad \mathbf{A}_3=\mathbf{a}_3\,. \qquad (1.\,8)$$

$\mathbf{k}=[\frac{1}{2}\frac{1}{2}\frac{1}{2}]$. Here according to (1. 6*a*), not only $2\mathbf{a}_1$, $2\mathbf{a}_2$ and $2\mathbf{a}_3$, but also $\mathbf{a}_1+\mathbf{a}_2$, $\mathbf{a}_2+\mathbf{a}_3$ and $\mathbf{a}_3+\mathbf{a}_1$, are translations of positive character so that a *F* lattice in the *B* notation is obtained (in the orthorhombic and cubic systems).

F lattices are not generally used in the tetragonal system so that by the transformation (1. 9) one arrives at the unit cell

$$\mathbf{A}_1=\mathbf{a}_1+\mathbf{a}_2;\quad \mathbf{A}_2=\mathbf{a}_1-\mathbf{a}_2;\quad \mathbf{A}_3=2\mathbf{a}_3 \qquad (1.\,9)$$

which is centred *I* in the B notation. Indeed the translation $\frac{1}{2}\mathbf{A}_1+\frac{1}{2}\mathbf{A}_2+\frac{1}{2}\mathbf{A}_3=\mathbf{a}_1+\mathbf{a}_3$ has positive character.

Another special case is the rhombohedral system in which one does not use the *F* centring in the unit cell $2a_1, 2a_2, 2a_3$ of volume $8\mathbf{a}_1\mathbf{a}_2\mathbf{a}_3$, but the simpler rhombohedral cell of volume $2\mathbf{a}_1\mathbf{a}_2\mathbf{a}_3$ with lattice translations

$$\mathbf{A}_1=\mathbf{a}_2+\mathbf{a}_3;\quad \mathbf{A}_2=\mathbf{a}_3+\mathbf{a}_1;\quad \mathbf{A}_3=\mathbf{a}_1+\mathbf{a}_2\,, \qquad (1.\,10)$$

which is why the B symbol is still *R*.

To summarize, maximal isoclass subgroups of index two of *P* lattices can be of type *P*, *C* and *F*, but not *I*, except in the tetragonal case where *F* transforms to *I* [*cf.* (1. 9] and in the monoclinic case where *C* transforms to *I* and *vice versa* by the transformations $\mathbf{A}_1=\mathbf{a}_1+\mathbf{a}_3$; $\mathbf{A}_2=\mathbf{a}_2$; $\mathbf{A}_3=-\mathbf{a}_3$ with $\mathbf{a}_j$ for the *C* cell and $\mathbf{A}_j$ for the *I* cell ($j=1,2,3$). Of course *C* centring can be made equivalent to *A* or *B* centring by a convenient change of axes.

Case 2. *The unit cell a_1, a_2, a_3 belongs to a centred lattice*

There are only two cases present in Table 1, both belonging to *C*.

The vector $\mathbf{k}=[00\frac{1}{2}]$ gives rise to a doubling in the $\mathbf{a}_3$ direction so the unit cell conserves the *C* type (C_{2c} in the OG and *C* in the B notation) in the orthorhombic and monoclinic systems.

The second case is that of $\mathbf{k}=[10\frac{1}{2}]$. It is seen from (1.6.*a*) that $\frac{1}{2}\frac{1}{2}0$ is an antitranslation, but that $\frac{1}{2}\frac{1}{2}1$ in the chemical cell, say $\frac{1}{2}\frac{1}{2}\frac{1}{2}$ in the cell $a_1, a_2, 2a_3$ is a translation of positive character, so the new cell is *I* centred (*cf.* Table 1 for the orthorhombic case).

To summarize, *C* lattices have isoclass subgroups of index two with the increased unit cell $a_1, a_2, 2a_3$ of lattices *C* and *I* only.

F and *I* lattices cannot have subgroups of index two with increased unit cells.

Remark. **k**-vectors which are not listed in Table 1 are of two kinds. They are either forbidden or equivalent, by a change of axes, to those already listed.

Thus $\mathbf{k}=[\frac{1}{2}00]$ is not listed for the tetragonal and cubic systems, because a unit cell $2a_1, a_2, a_3$ cannot be of the same class (neither tetragonal, nor cubic).

$\mathbf{k}=[\frac{1}{2}0\frac{1}{2}]$ is not listed in the monoclinic system; in the new equivalent axes (spanning the same unit-cell volume) $\mathbf{A}_1=\mathbf{a}_1$; $\mathbf{A}_2=\mathbf{a}_2$; $\mathbf{A}_3=\mathbf{a}_1+\mathbf{a}_3$, the wavevector becomes $\mathbf{k}_1=[\frac{1}{2}00]$ which is listed in Table 1. The same reduction procedure is valid in the triclinic system. For the same reasons $\mathbf{k}=[10\frac{1}{2}]$ is not of general use in the monoclinic system (in other words C_I in the OG and I_c in the B notation are not listed) because here the anticentred *C* lattice can always be transformed into a centred *C* lattice by the transformation to the new equivalent axes $\mathbf{A}_1=\mathbf{a}_1+2\mathbf{a}_3$, $\mathbf{A}_2=\mathbf{a}_2$; $\mathbf{A}_3=2\mathbf{a}_3$ for which the wave vector becomes $\mathbf{k}_1=[00\frac{1}{2}]$. Also note that $C_a=C_b$ in the B notation.

I. 4. *Space groups*

Here again we first recall matters of notation which are important for our purpose.

In the OG notation symmetry elements are noted by their Hermann–Mauguin symbols, antisymmetry elements (excepting antitranslation) by primed symbols. The same is true in the B notation. Thus both notations are identical in all cases where chemical and magnetic translation lattices coincide, but differ as soon as an antitranslation is present. Here OG continue to use unprimed and primed Hermann–Mauguin symbols in the chemical cell preceded by a capital letter which characterizes the lattice type of the chemical cell and a subscript which indicates the new periodicity while B uses *exclusively* unprimed Hermann–Mauguin symbols (no antisymmetry element present) preceded by the symbol of the translation lattice in the new unit cell and a subscript which describes the antitranslation.

Thus we retain in the OG symbol the space group *G* (suppressing all primes) and the new periodicity (which is also apparent from the **k** vectors of Table 1) while the B symbol, suppressing the subscript of the antitranslation, gives us directly the maximal subgroup *H* for which we look and contains only symmetry elements. In other words, in the magnetic space groups G_m [*cf.* relation (1. 2)], the B notation is just $H_{g'}$ where *H* is the maximal subgroup of *G* and g' is the antitranslation symbol.

Finally, our problem is reduced to transforming the known OG symbols (with translation lattices listed in Table 1) to the corresponding B symbols. This is done in the following steps.

(1) Note the space group G to which the OG symbol belongs and the new unit cell from the subscript or from the **k** vector.

(2) Read from Table 1 the translation lattice in the new unit cell (B symbol) and the antitranslation subscript.

(3) Conserve the unprimed Hermann–Mauguin symmetry elements; multiply each primed element by the antitranslation. The result is an (unprimed) symmetry element which one substitutes for the primed one.

(4) In the B symbol thus obtained suppress the subscript to obtain the maximal subgroup H of G; eventually transform the B symbol to the standard setting used in *International Tables for X-ray Crystallography* (1952) and in the OG and B tables.

Example 1. *OG symbol* $P_{2b}m'ma$

Step 1. The space group is *Pmma*, the increased unit cell is $a_1, 2a_2, a_3$; the **k** vector is $[0\frac{1}{2}0]$.

Step 2. To P_{2b} corresponds P_b(B); $b=(a_2)'$ is an antitranslation.

Step 3. The multiplication of the antisymmetry plane m'_x by the antitranslation $(a_2)'$ gives rise to a glide plane b_x in the new unit cell:

$$m'_x \times (a_2)' = m_x \times a_2 = b_x \, .$$

Step 4. The B symbol is P_bbma. Thus the space group $G=Pmma$ (unit cell a_1, a_2, a_3) has a maximal subgroup $H=Pbma$ (unit cell $a_1, 2a_2, a_3$).

Remark. The standard setting is not *bma* but *bcm* (see (*International Tables*, 1952, p. 548). Indeed by the circular permutation $x \rightarrow y \rightarrow z \rightarrow x$, one has $a_z \rightarrow b_x$, $m_y \rightarrow m_z$, $b_x \rightarrow c_y$, $b \rightarrow c$ so that $P_bbma \doteq P_cbcm$ (wrongly given as P_bbcm in OG). Table 3 summarizes the maximal subgroups H with increased unit cell of the orthorhombic P space group $G=Pmma$. The first and second columns contain the magnetic space groups G_m in the OG and corresponding B notation respectively. The third column indicates the increased cell dimensions. The last column repeats the B symbol in its standard notation when that of the second column is different. The maximal subgroup H of G is read from the second column, suppressing the subscript (or just interpreting it as being the cell dimension to be increased).

Remark on tabulations. Opechowski & Guccione (1965) have tabulated the magnetic groups G_m in the OG *and* in the B standard notation. Their tables can be used for all the systems with the sole exception of the orthorhombic system where the B symbol derived from the OG symbol by the procedure described above differs sometimes from the standard notation. The author has also tabulated the maximal subgroups of the orthorhombic system in a way similar to Table 3.*

Neubüser & Wondratschek (1966) have derived diagrams of space group–subgroup relations for the classes 23, $m\bar{3}$, 432 and $\bar{4}3m$, the isoclass subgroups being of indices two and four. Also a tabulation of subgroups (Neubüser & Wondratschek, 1970) was circulated among the members of the IUCr Commission on *International Tables*. This tabulation, derived from a computer program, comprised a great number of maximal subgroups of index two. However those space groups for which the maximal subgroup H has the same Hermann–Mauguin symbol were omitted.

Actually there are 1421 magnetic space groups from which one may derive 1191 maximal subgroups H of index two of the 230 space groups G. There are 674 isotranslation subgroups [category (*a*) of the *Introduction*] and 517 isoclass subgroups [category (*b*)] corresponding to the 517 magnetic groups with antitranslations and falling into two categories. There are 329 subgroups H with increased unit cells [category (*b*1); translation lattices of Table 1] and 188 with the same unit cell, but with partial or total loss of centring [category (*b*2); translation lattices of Table 2]. The categories (*b*1) and (*b*2) correspond to magnetic space groups G_m with integer and fractional antitranslations respectively.

Among the 329 maximal subgroups H with increased unit cells there is an important fraction of 99 subgroups, tabulated in Table 4 where H and G have the same Hermann–Mauguin symbol. Clearly $H \sim G$ where $\sim$ means isomorphous with. These 99 subgroups H fall into two sets: 54 are derived from (44) symmorphous space groups and 45 belong to (40) non-symmorphous space groups G. The reasons for $H \sim G$ will appear later (see § II. 1. 5).

* These tables are available as photocopies which may be purchased from the author or obtained from the deposit with the British Library Lending Division, Supplementary Publication No. 31933 (8 pp.), through The Executive Secretary, International Union of Crystallography, 13 White Friars, Chester CH1 1NZ, England.

Table 3. *Connexion between magnetic space groups and maximal subgroups H of a space group G. Example*: $G=Pmma$

OG is Opechowski–Guccione, B is Belov notation of magnetic groups. The subgroups H are read from the second column, suppressing the subscript and using the increased cell dimension(s) of the third column.

OG	B	Increased dimension	B standard notation	OG	B	Increased dimension	B standard notation
$P_{2b}mma$	P_bmma	2*b*		$P_{2b}m'ma'$	P_bbmn	2*b*	P_abmn
$P_{2c}mma$	P_cmma	2*c*		$P_{2c}m'ma$	P_ccma	2*c*	P_abam
P_Amma	A_bmma	2*b*, 2*c*	C_amcm	$P_{2c}mm'a$	P_cmca	2*c*	P_bbcm
$P_{2b}m'ma$	P_bmma	2*b*	P_cbcm	$P_{2c}m'm'a$	P_ccca	2*c*	
$P_{2b}mma'$	P_bmmn	2*b*	P_ammn	$P_Am'ma$	A_ccma	2*b*, 2*c*	C_amca

Remark on the isoclass subgroups of category (*b*2). The procedure of four steps outlined above applies to any magnetic space group G_m with antitranslations. As an example consider *Ccca* where the following four anticentred groups G_m exist: C_Pcca, $C_Pc'ca$, $C_Pcc'a$, and $C_Pc'c'a$ in the OG notation. The transformation to B symbols yields (see also Bertaut, 1975*a*) *Pcca*, *Pnca*, *Pcna* and *Pnna*.

Remark on equivalencies. The direct procedure outlined for maximal *P* subgroups of *C* and *I* groups (Bertaut, 1976) obtains these plus four more groups, *Pncb*, *Pcnb*, *Pccb* and *Pnnb*, but they are equivalent to the preceding ones. The reader must keep in mind indeed that only the non-equivalent magnetic groups are tabulated. Equivalency relations in magnetic space groups have been given (Bertaut, 1975*b*). Their tabulation is equivalent to and even more informative than the tabulation of magnetic space groups.

Remark on isotranslational subgroups [*category* (*a*)]. Although relation (1. 1) is generally used to construct maximal isotranslation subgroups, it is possible to reconstruct them from magnetic space groups without antitranslations.

Example 1. *Pc'ca*. The product c_ya_z is equivalent to 2_{1x}. Thus $Pc'ca=H+c'_xH$ with $H=P2_1ca$.

Example 2. *Pc'c'a*. The product $c'_x \cdot c'_y$ is equivalent to 2_z. Thus $Pc'c'a=H+c'_xH$ with $H=P2_z/a$.

As a classroom example, the reader may check again that equivalency relations between magnetic groups G_m (Bertaut, 1975*b*) correspond to equivalent subgroups *H*.

Part II. Direct approach

Although a detour through the (already tabulated) magnetic space groups is comfortable, one might look for a more direct approach. We shall state here the cases which are to be excluded, *i.e.* we state the rules under which a space group *G* has no maximal subgroup *H*.

II. 1. *Maximal subgroups of index two*

We write again relation (1. 1) in the form appropriate for our purpose

$$G=H+(e|\mathbf{t}_G)H \qquad (2.\ 1)$$

where $\mathbf{t}_G$ is a lattice translation of *G*, not contained in *H*. *H* only contains the even powers of $(e|\mathbf{t}_G)$.

The closure property, *H* is a group, implies that any combination of elements of *H* must be again in *H*, and cannot be in $(e|\mathbf{t}_G)H$.

Rule 1. An element $(\beta|\tau_\beta)$ of *G* cannot be in *H* if a power $(\beta|\tau_\beta)^n$ is equal to the translation $(e|\mathbf{t}_G)$ or to an odd power of $(e|\mathbf{t}_G)$ or, expressed otherwise, if *G* contains elements $(\beta|\tau_\beta)$ whose power is equal to $(e|\mathbf{t}_G)$ no maximal subgroup *H* can be found containing $(\beta|\tau_\beta)$ and satisfying (2. 1).

Rule 2. If there are two elements of *G*, say $(\alpha|\tau_\alpha)$ and $(\beta|\tau_\beta)$ whose combination by group operations results in a lattice translation $(e|\mathbf{t}_G)$, these two elements cannot be simultaneously in *H*.

II. 1. 1. *Screw axes*

One has

$$(n_m)^n=m\mathbf{t}\,. \qquad (2.\ 2)$$

Axes n_m with *m* odd, present in *G*, exclude the decomposition (2. 1), *i.e.* do not allow doubling of the unit cell in the direction **t** of the rotation axis. Thus, axes $2_1, 3_1, 4_1, 4_3, 6_1, 6_3, 6_5$, cannot be present in *G and H* for this case. (The case of 3_1 will be considered again below).

Axes n_m with *m* even, present in *G*, are allowed; one must only keep in mind that an axis n_m in *G* becomes $n_{m/2}$ in *H*. Thus 3_2 in *G* becomes 3_1 in *H* with the same handedness.

The case of 3_1 needs special care. As already stated, 3_1 cannot be simultaneously in *H* and in *G*. Consider however the even powers of 3_1 in *G*. The first even power which gives rise to a rotation of $120°=(2\pi)/3$ is $(3_1)^4$. The translational component is $(4/3)\mathbf{t}_G$ in *G* and $(2/3)\mathbf{t}_H$ in *H* with $\mathbf{t}_H=2\mathbf{t}_G$. Thus the action of $(3_1)^4$ in *G* is equivalent to that of $(3_2)^1$ in *H*. It is then an easy matter to see that the powers $(3_1)^p$ in *G* with *p* even are equivalent to the action of powers of 3_2 in *H*, whilst powers $(3_1)^p$ in *G* with *p* odd are equivalent to the action of powers of 3_2 in *H plus* a translation $\mathbf{t}_G$.

Thus the decomposition (2. 1) *is* possible, 3_1 in *G* becoming 3_2 in *H*.

II. 1. 2. *Glide planes*

a, *b* and *c* planes in *G* do not allow doubling of the unit cell in the **x**, **y** and **z** directions respectively.

An *n* plane perpendicular to *Ox* is compatible with doubling the unit cell in the *Oy* and *Oz* directions simultaneously, but incompatible with doubling in only one of these directions.

Note that under these circumstances, an *n* plane in *G* becomes a *d* plane in *H*.

Remark. *d* planes only exist in *F* and *I* lattices [they are such that $d^2=(e|\mathbf{t}_d)$ with $\mathbf{t}_d$ a fractional translation] which do not admit maximal subgroups *H* of order two.

II. 1. 3. *Applications of rule* 1

Example 1. *Pmma*. The full symbol is $P2_1/m\ 2/m\ 2/a$. The presence of the glide plane *a* as well as of the helical axis 2_1 excludes doubling of the unit cell along *Ox*. Doubling along *Oy* and/or *Oz* is allowed. We only work out the maximal subgroups for the unit cell a_1, $2a_2, a_3$. The plane m_x either remains m_x or becomes b_x; the plane m_y remains m_y; the plane a_z either remains a_z or becomes n_z. Thus there are four maximal subgroups possible with the unit cell $a_1, 2a_2, a_3$: *Pmma*, *Pbma*, *Pmmn*, *Pbmn*. The reader may work out the maximal subgroups of *Pmma* and check the results of Table 3.

Example 2. $P4/nnc$ and $Pnma=P2_1/n\ 2_1/m\ 2_1/a$. The binary elements exclude any doubling in any direction.

II. 1. 4. *Applications of rule* 2

Rule 2 will be needed only in a non-symmorphous space group, having a centre of symmetry which we suppose is located at the origin. With the elements $(\bar{1}|000)$ and $(\alpha|\tau_\alpha)$ one constructs the products $(\alpha\,.\,\bar{1}|\tau_\alpha)$ and $(\bar{1}\,.\,\alpha|-\tau_\alpha)$ and the squares $[\alpha^2|(\alpha+e)\tau_\alpha]$, $(\alpha\,.\,\bar{1}|\tau_\alpha)^2 = [\alpha^2|(e-\alpha)\tau_\alpha]$ and $(\bar{1}\,.\,\alpha|-\tau_\alpha)^2 = [\alpha^2|(\alpha-e)\tau_\alpha]$ which have the same rotational part. Consequently, according to rule 2 the differences of their translational parts, *i.e.* $2\tau_\alpha$ and $2\alpha\tau_\alpha$, should not be equal to $\mathbf{t}_G$, but should remain translations of H, to be allowed. In the **k**-formalism this means that

$$\exp(2\pi i\mathbf{k}\,.\,2\tau_\alpha) = +1 \quad \text{and} \quad \exp(2\pi i\mathbf{k}\,.\,2\alpha\tau_\alpha) = +1\,.$$

Example 1: $P4_2/n$. Here $\tau_\alpha = 0\frac{1}{2}\frac{1}{2}$; $\alpha = 4_z$; $2\tau_\alpha = 011$ and $2\alpha\tau = -101$. Only $\mathbf{k} = [\frac{1}{2}\frac{1}{2}\frac{1}{2}]$, *i.e.* increase in the three dimensions simultaneously is allowed. In the unit cell $2a_1, 2a_2, 2a_3$, 4_2 becomes 4_1 and $n = (m_z|\frac{1}{2}\frac{1}{2}0)$ becomes $(m_z|\frac{1}{4}\frac{1}{4}0)$ which according to the change of axes (1. 9) transforms to $(m_z|\frac{1}{2}00)$, *i.e.* to an *a* plane. Thus the (only) isoclass maximal subgroup is $I4_1/a$.

Example 2: $P4/n$. Here $\tau_\alpha = \frac{1}{2}00$; $2\tau_\alpha = 100$ and $2\alpha\tau_\alpha = 010$. Only doubling along the *c* axis is allowed. The maximal subgroup in the new unit cell $a_1, a_2, 2a_3$ is still $P4/n$.

II. 1. 5. *The case* $H \sim G$

Symmorphous groups. Rules 1 and 2 do not apply. One must however exclude *F* and *I* lattices which do not admit isoclass subgroups of index two in a unit cell increase and cubic *P* lattices which would give rise to *F* lattices.

Non-symmorphous groups. Here it is required that the directions in which the unit cell is increased are orthogonal to the fractional translations of the screw axes and/or glide planes present (Table 4).

II. 2. *Maximal isoclass subgroups of index four*

Let *G* be a group and *H* a maximal subgroup of *G* of index 4.

$$G = H + g_1H + g_2H + g_3H \qquad (2.\,3)$$

where g_j $(j = 1,2,3)$ is in *G*, but not in *H*.

II. 2. 1. *Same unit cell*

A simple example is provided by cubic space groups *G* with *F* lattices and subgroups *H* with *P* lattices of the same unit cell (category *b*2) with $g_1 = \frac{1}{2}\frac{1}{2}0$, $g_2 = \frac{1}{2}0\frac{1}{2}$, $g_3 = 0\frac{1}{2}\frac{1}{2}$. For instance in $Fm3m$, the *m* planes perpendicular to the *x*, *y*, *z* axes are associated with the *n* planes through the fractional translations g_j. Thus the above decomposition with $G = Fm3m$ is valid for $H = Pm3m, Pn3m$ (but not for $Pm3n$ and $Pn3n$). For $G = Fm3c$ one has $H = Pm3n$ and $Pn3n$. *F* lattices with *d* planes do not admit an isoclass decomposition following (2. 3). One easily completes the list of maximal isoclass subgroups of index four with $G = F23$, $H = P23$ and $P2_13$; $G = Fm\bar{3}$, $H = Pm\bar{3}$ and $Pa\bar{3}$; $G = F432$, $H = P432$ and $P4_232$; $G = F\bar{4}3m$, $H = P\bar{4}3m$; $G = F\bar{4}3c$, $H = P\bar{4}3n$.

In orthorhombic groups *G* with *F* lattices the decomposition (2. 3) is possible (except when *d* planes are present), but *H* is no longer a maximal subgroup. Indeed from (2. 4) follows (2. 5) where $K = H + g_1H$ is a maximal subgroup (*C* lattice)

$$g_2 = g_3g_1 \qquad (2.\,4)$$

$$G = (H + g_1H) + g_3(H + g_1H) = K + g_3K\,. \qquad (2.\,5)$$

II. 2. 2. *Increased unit cell*

P lattices have no maximal *I* subgroups of index two (excepting the tetragonal and monoclinic cases mentioned in § I. 3). Thus we suspect that a *P* lattice might have an *I* lattice as maximal subgroup of order four. One has indeed

$$P = I + (e|\mathbf{a}_1)I + (e|\mathbf{a}_2)I + (e|\mathbf{a}_3)I\,. \qquad (2.\,6)$$

Here *P* is the translation lattice of unit cell $\mathbf{a}_1, \mathbf{a}_2, \mathbf{a}_3$ and *I* the translation lattice of unit cell $2\mathbf{a}_1, 2\mathbf{a}_2, 2\mathbf{a}_3$ which contains eight points as follows, referred to the *P* lattice,

(000; 111); (100; 011); (010; 101); (001; 110).

They become, referred to the *I* lattice,

$(000; \frac{1}{2}\frac{1}{2}\frac{1}{2})$; $(\frac{1}{2}00; 0\frac{1}{2}\frac{1}{2})$; $(0\frac{1}{2}0; \frac{1}{2}0\frac{1}{2})$; $(00\frac{1}{2}; \frac{1}{2}\frac{1}{2}0)$

and represent exactly the decomposition (2. 6) above.

Table 4. *Maximal subgroups H of G with* $H \sim G$

The subscripts *a*, *b*, *c* indicate a unit-cell doubling in the **a**, **b**, **c** directions respectively; *s* stands for doubling in any direction and subscript *C* stands for the increased unit cell $a\sqrt{2}, a\sqrt{2}, c$.

Symmorphous groups	
Triclinic	P_s1; $P_s\bar{1}$
Monoclinic	
(*b* unique axis)	P_a2; P_b2; C_c2; P_am; P_bm; C_cm; P_a2/m; P_b2/m; C_c2/m
Orthorhombic	P_s222; C_c222; P_cmm2; P_ammm2; C_cmm2; A_ammm2; P_smmm; C_cmmm
Tetragonal	P_c4; P_C4; $P_c\bar{4}$; $P_C\bar{4}$; P_c4/m; P_C4/m; P_c422; P_C422; P_c4mm; P_C4mm; $P_c\bar{4}2m$; $P_C\bar{4}m2$; P_c4/mmm; P_C4/mmm
Trigonal	P_c3; R_c3; $P_c\bar{3}$; $R_c\bar{3}$; P_c312; P_c321; R_c32; P_c3ml; P_c31m; R_c3m; $P_c\bar{3}1m$; $P_c\bar{3}ml$; $R_c\bar{3}m$
Hexagonal	P_c6; $P_c\bar{6}$; P_c6/m; P_c622; P_c6mm; $P_c\bar{6}m2$; $P_c\bar{6}2m$; P_c6/mmm
Non-symmorphous groups	
Monoclinic	
(*b* unique axis)	P_a2_1; P_ac; P_bc; P_a2_1/m; P_a2/c; P_b2/c; P_a2_1/c
Orthorhombic	P_a222_1; $P_c2_12_12$; P_amc2_1; P_bmc2_1; P_acc2; P_bma2; P_cma2; P_bca2_1; P_anc2; P_bmn2_1; P_cba2; A_abm2; P_accm; P_cban; P_bmma; P_cmma; P_bmna; P_bcca; P_cbam; P_abcm; P_cmmn; C_cmma
Tetragonal	P_C4_1; P_C4_2; P_C4_3; P_C4_2/m; P_c4/n; P_c42_12; P_C4_122; P_C4_222; P_C4_322; P_c4bm; P_C4cc; $P_c\bar{4}2_1m$; $P_c\bar{4}b2$; P_C4/mcc; P_c4/nbm; P_c4/mbm

Consider (2. 3) where G is a space group with a P lattice, H a subgroup with an I lattice, g_j being the translation $(e|\mathbf{a}_j)$ and again ask the question of the symmetry elements which cannot be in G *and* in H simultaneously. We first discuss cubic space groups. Glide planes a,b,c must be excluded. Indeed a cannot be in H because $(a)^2=(e|\mathbf{a}_1)$ would be in the second coset of (2. 3). Glide planes n, orthogonal to the axes, must be excluded. An example is $n_x^2=(e|\mathbf{a}_2)+(e|\mathbf{a}_3)$ which are in the third and fourth cosets. However, diagonal n planes which occur in cubic lattices are allowed. They are such that

$$n^2=(e|\mathbf{a}_1+\mathbf{a}_2+\mathbf{a}_3)=1,1,1 \text{ in the primitive unit cell}$$

and

$$=\tfrac{1}{2},\tfrac{1}{2},\tfrac{1}{2} \text{ in the unit cell } 2a_1,2a_2,2a_3\,. \qquad (2.\ 7)$$

Thus the n plane in the P cell becomes a d plane in the I cell. Axes $2_1,4_1,4_3$ are excluded, while 4_2 is allowed. Maximal subgroups of index four are cubic. They are summarized in Table 5(*a*).

Table 5. *Subgroups of index four* (*I lattices*)

(*a*) Cubic space groups

The subgroups H of index four are maximal.

$G(a_1a_2a_3)$	$H(2a_1,2a_2,2a_3)$	G	H
$P23$	$I23$	$P4_232$	$I4_132$
	$I2_13$	$P\bar{4}3m$	$I\bar{4}3m$
$Pm\bar{3}$	$Im\bar{3}$	$P\bar{4}3n$	$I\bar{4}3d$
	$Ia\bar{3}$	$Pm\bar{3}m$	$Im\bar{3}m$
$P432$	$I432$	$Pm\bar{3}n$	$Ia\bar{3}d$

(*b*) Orthorhombic space groups

The subgroups H of index four are not maximal; they are maximal subgroups of index two of the respective C groups, $C222$, $Cmm2$ and $Cmmm$.

$G(a_1a_2a_3)$	$H(2a_1,2a_2,2a_3)$	G	H
$P222$	$I222$	$Pmmm$	$Immm$
	$I2_12_12_1$		$Imma$
$Pmm2$	$Imm2$		$Ibam$
	$Ima2=Ibm2$		$Ibca$
	$Iba2$		

Of course, in the orthorhombic system the derivation of all possible subgroups H of index four and lattice I from a space group G of lattice P follows the same lines, *i.e.* one must exclude glide planes a,b,c,n in G. However these subgroups H, listed in Table 5(*b*) are no longer maximal because one has the relations (2. 8) (*cf.* § I. 3, case 2) and (2. 9):

$$C=I+(e|\mathbf{a}_3)I \qquad (2.\ 8)$$

$$P=C+(e|\mathbf{a}_1)C\,. \qquad (2.\ 9)$$

Here the unit cells are a_1,a_2,a_3 in P; $2a_1,2a_2,a_3$ in C; $2a_1,2a_2,2a_3$ in I.

Conclusions

The author would like to emphasize two main conclusions. The first one is about the potential importance of group–subgroup relations (see also Neubüser & Wondratschek, 1966). Bärnighausen (1975) has recently constructed a 'family tree' of such group–subgroup relations in the perovskite family which provides an interesting synoptic ordering principle, relating the high-symmetry to the low-symmetry compound by a sequence of maximal isotranslational and/or isoclass subgroups. Further investigations have to show if such a family tree is useful for distinguishing and predicting the nature of transitions (first or second order). Another example is provided by NbO_2 where the following stepwise sequence through maximal subgroups $P4_2/mnm$ $(a,a,c)\rightarrow P4_2/m$ $(a,a,c)\rightarrow P4_2/m$ $(a\sqrt{2},a\sqrt{2},c)\rightarrow P4_2/n$ $(2a,2a,c)\rightarrow I4_1/a$ $(2a\sqrt{2},2a\sqrt{2},2c)$ leads from the high-temperature (rutile) to the low-temperature form with a 16-fold increase of the unit cell (Marinder, 1963). The question is whether the stepwise sequence corresponds to a stepwise reaction or not. In the present example there are clear indications (Shapiro, Axe, Shirane & Raccah, 1974) that the transition is in one step from $P4_2/mnm$ to $I4_1/a$, *i.e.* to a subgroup of index 16.

The second point is that no field of symmetry considerations should leave the crystallographer indifferent even if at first sight it only seems to represent an interest for a limited number of people. This is clearly exemplified by the connexion shown to exist (Part 1) between magnetic space groups with integer antitranslations and maximal subgroups of index two with increased unit cell.

Comments

In a very positive referee's report the attention of the author was drawn to the paper *Klassengleichen Supergroup–Subgroup Relations Between the Space Groups* (Boyle & Lawrenson, 1972) in which the volume ratios of the unit cells of 'Klassengleiche' (isoclass) subgroups H and groups G are tabulated, but without distinguishing maximal and non-maximal subgroups. Such tables are surely useful for the physicist. Still, this paper is able to clear ambiguities and also provides a useful means for checking the validity of their tabulation for maximal subgroups.

For instance we read either from our direct approach (Part II) or from the Opechowski–Guccione tables that $P4/mmm$-D_{4h}^1 (unit cell a,a,c) has the following maximal isoclass subgroups:

$P4/mmm$-D_{4h}^1; $P4/nbm$-D_{4h}^3; $P4/mbm$-D_{4h}^5; $P4/nmm$-D_{4h}^7 with the unit cell $a\sqrt{2},a\sqrt{2},c$; B notation P_C.

$P4/mmm$-D_{4h}^1; $P4/mcc$-D_{4h}^2; $P4_2/mmc$-D_{4h}^9; $P4_2/mcm$-D_{4h}^{10}; $P4_2/nbc$-D_{4h}^{11} with the unit cell $a,a,2c$; B notation P_c.

$I4/mmm$-D_{4h}^{17}; $I4/mcm$-D_{4h}^{18} with the unit cell $a\sqrt{2}$, $a\sqrt{2},2c$; B notation I_c.

The Boyle–Lawrenson tables cannot distinguish dif-

ferent cases of doubling the unit-cell volume, for instance doubling in the **c** direction or in the *c* plane as exemplified above.

Also, in their Table 5 a minimum volume ratio of eight is assigned to the subgroups D_{4h}^5, D_{4h}^7, D_{4h}^9, D_{4h}^{10} and of four to the subgroup D_{4h}^{11} of the space group D_{4h}^1 whilst according to the example above this volume ratio is two. (No other errors have been found however.)

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Neutron Small-Angle Scattering by Dislocations in Homogeneously Oriented Nematic Liquid Crystals

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A complete examination of the shape of the neutron-scattering cross-section curves at very small scattering vectors, of the order of $0{\cdot}05 \sim 0{\cdot}1$ nm^{-1}, has been made for homogeneously oriented nematic liquid crystals. It is shown that the shape of the scattering curves at small angles is mainly determined by the kind of dislocation configuration exhibited by homogeneously oriented nematic liquid crystals. This study will furnish a partial guide to the construction of scattering relations for any kind of possible dislocation configuration in homogeneously oriented nematic liquid crystals, *e.g.* for stationary straight edge dislocations, moving edge dislocations, oscillating edge dislocations, curved dislocations and dislocation networks.

1. Small-angle scattering of neutrons and X-rays by dislocations in homogeneously oriented nematic liquid crystals

In a previous paper (Olivei, 1973) we have already discussed the usefulness of using cold-neutron scattering for probing the molecular structure of homogeneously oriented nematic liquid crystals in the absence of any external magnetic or electric fields. In that paper, however, we did not examine the cold-neutron scattering at very small values of the scattering vector (of the order of $0{\cdot}05 \sim 0{\cdot}1$ nm^{-1}). In fact, such a study should yield very interesting results about the existence and the structure of dislocations in homogeneously oriented nematic liquid-crystal layers.

The existence of lines or regions of discontinuity in the ordered structure of homogeneously oriented nematic liquid-crystal layers makes possible the setting up of dislocations of various kinds.

The use of cold-neutron small-angle scattering for studying dislocations in homogeneously oriented nematic liquid-crystal structures has advantages as compared to X-ray scattering. In principle, small-angle scattering of X-rays and neutrons is induced by long-range fluctuations of density or refractive index in a sample. Such fluctuations are produced by many types of structural disorder, *e.g.* dislocations, defect clusters, critical phenomena.

The first advantage of neutrons as compared to X-rays concerns the change of the wavelength. In most