Acta Cryst. (1996). A52, 681–685

Maximal Subgroups of Magnetic Space Groups and Subperiodic Groups

DANIEL B. LITVIN

Department of Physics, The Pennsylvania State University, Penn State Berks Campus, PO Box 7009, Reading, PA 19610-6009, USA

(Received 10 October 1995; accepted 2 April 1996)

Abstract

An algorithmic procedure is presented to determine the maximal subgroups of magnetic space groups and subperiodic groups from the maximal subgroups of non-magnetic space groups and subperiodic groups. As an example of the application of this procedure, the maximal subgroups of the magnetic frieze groups are derived and tabulated.

1. Introduction

Among the information provided in Volume A of *International Tables for Crystallography* (1983) [abbreviated here as ITC(1983)] on non-magnetic space groups are tabulations of the maximal subgroups of the space groups. In this paper, we set forth a procedure to derive the maximal subgroups of magnetic space groups. This procedure will be used (Litvin, 1996) in the compilation of information on magnetic groups in the format and content of ITC(1983). The knowledge of the maximal subgroups of magnetic groups, in particular, can be applied in the analysis of phase transitions in magnetic materials (Cracknell, 1975). This procedure is also valid for magnetic crystallographic subperiodic groups, *i.e.* magnetic layer, rod and frieze groups.

In §2, we review Hermann's (1929) theorem on subgroups of space groups and the classification of maximal subgroups used in ITC(1983). In §3, we set out a procedure to derive the maximal subgroups of magnetic space groups and subperiodic groups. In §4, as an example, we derive the maximal subgroups of the magnetic frieze groups.

2. Maximal subgroups

Hermann's theorem (Hermann, 1929; see also Opechowski, 1986) states that every subgroup of a space group **G** is an equi-class subgroup of an equi-translational subgroup of **G**. It follows that every maximal subgroup of a space group **G** is either a maximal equi-class subgroup or a maximal equi-translational subgroup. The ITC(1983) classification of maximal subgroups of space groups is based on this fact.

Consequently, the ITC(1983) classification classifies the maximal subgroups into two types: type I, equi-translational (*translationengleiche*) maximal subgroups; and type II, equi-class (*klassengleiche*) maximal subgroups.

In addition, there is the subclassification into (i) maximal non-isomorphic non-enantiomorphic subgroups, and (ii) maximal isomorphic and enantiomorphic subgroups. As the number of maximal isomorphic and enantiomorphic subgroups is infinite, only those of lowest index are explicitly given [ITC(1983)].

For space groups, the terminology 'isomorphic' can be used for the longer expression 'belonging to the same type (class)' and is justified through Bieberbach's (1912) theorem. Since Bieberbach's theorem is not valid for subperiodic groups, we cannot use this terminology when considering subperiodic groups. As we derive a single procedure for determining the maximal subgroups of both magnetic space groups *and* subperiodic groups, we shall use the terminology *isotypic* for the longer expression 'belonging to the same type (class)'. In this new terminology, the subclassification is (i) maximal non-isotypic non-enantiomorphic subgroups, and (ii) maximal isotypic subgroups and enantiomorphic subgroups of lowest index.

Following ITC(1983), the complete classification of maximal subgroups **S** of space groups **G** is then:

Maximal non-isotypic non-enantiomorphic subgroups: I maximal equi-translational subgroups; II*a* maximal equi-class subgroups where the conventional unit cells of **G** and **S** are the same; II*b* maximal equi-class subgroups where the conventional cell of **S** is larger than that of **G**. Maximal isotypic and enantiomorphic subgroups of lowest index: II*c* maximal equi-class subgroups.

We note that in ITC(1983) every maximal subgroup **S** of **G** of types I and II*a* are explicitly listed. For type II*b* and II*c* subgroups, one entry there may correspond to more than one subgroup. One entry may correspond to subgroups whose differences can be expressed as different conventional origins of **S** with respect to **G**

ISSN 0108-7673

or with cell enlargements in different directions (see also Billiet, 1981).

3. Maximal subgroups of magnetic groups

Let **G** denote a space group or subperiodic group and **1′** the time inversion group consisting of two elements, identity, 1, and time inversion, 1′. **G1′** will denote the group that is the direct product of **G** and **1′**. We will denote by **G[H]** the group where all elements of **G** not contained in the subgroup **H** of index 2 are multiplied by time inversion.

To obtain a survey of all magnetic space groups or subperiodic groups, one begins by listing, *e.g.* for magnetic space groups, one *representative* space group **G** from each type of space group. That is, one chooses from all the space groups belonging to this space-group type a single specific space group to be included in the survey. For each group **G**, one adds to this list the group **G1′** and one representative group **G[H]** from each type of group of this form. A list of the groups **G**, **G1′** and **G[H]** for a specific group **G** is referred to as the *reduced magnetic superfamily* of **G** (Opechowski, 1986). A survey of all magnetic space groups or subperiodic groups consists of a listing of the reduced magnetic superfamilies of all the space groups or subperiodic groups. We shall refer to such a list simply as 'the list of magnetic space groups or subperiodic groups'.

A procedure to find the maximal subgroups of magnetic space groups or subperiodic groups is as follows (a proof is given in Appendix *A*):

(i) The maximal subgroups **S** of **G** are determined and classified in types I, II*a*, II*b* and II*c*. We assume in the following steps that these maximal subgroups are known.

(ii) The maximal subgroups of **G1′** are:

(*a*) the group **G** is a maximal subgroup of **G1′** and is classified as a type I maximal subgroup;

(*b*) for each maximal subgroup **S** of **G**, **S1′** is a maximal subgroup of **G1′**. Each group **S1′** is classified as the same type of maximal subgroup as **S**;

(*c*) for each maximal subgroup $\mathbf{S}_2$ of index 2 in **G**, $\mathbf{G}[\mathbf{S}_2]$ is a maximal subgroup of **G1′**. Each group $\mathbf{G}[\mathbf{S}_2]$ is classified as a maximal subgroup of type I if $\mathbf{S}_2$ and **G** have the same translational subgroups and as type II*b* if not.

(iii) The maximal subgroups of **G[H]** are:

(*a*) **H** is a subgroup of index two of **G[H]** and consequently is a maximal subgroup;

(*b*) the remaining maximal subgroups of **G[H]** are determined as follows: (i) one determines the maximal subgroups $\mathbf{S}_G \neq \mathbf{H}$ of **G**; (ii) for each such maximal subgroup $\mathbf{S}_G$ one determines all subgroups **K**, of index two of $\mathbf{S}_G$, which are also subgroups of **H**. Each group $\mathbf{S}_G[\mathbf{K}]$ is a maximal subgroup of **G[H]**. As we shall show below, to determine the maximal subgroups of **G[H]** of type II*c* may require the knowledge of the type II*c* maximal subgroups of **G** beyond that of the lowest index.

4. Maximal subgroups of the magnetic frieze groups

Frieze groups are two-dimensional groups whose translational subgroup is one-dimensional. The seven types of frieze groups are listed in Table 1. In the first and second columns, we give, respectively, a sequential numbering and a symbol for each frieze-group type. Each frieze-group-type symbol will also be taken as the symbol for the representative frieze group which we consider and which is defined in each row of Table 1. The translational subgroup of each of these groups is $p = \langle(E|1,0)\rangle$, where $(E|1,0)$ denotes the translation that generates the translational subgroup. Each representative frieze group is defined by this translational subgroup and a set of coset representatives of the coset decomposition of the frieze group with respect to this translational subgroup. The coset representatives of each representative frieze group are listed, in Table 1, to the right of the symbol of that group.

There are 31 types of magnetic frieze group. These correspond to the 31 types of 'black and white' frieze groups where 1′ is interpreted as a color-reversing operation (Belov, 1956) and to the 31 types of 'anti-symmetry' frieze groups where 1′ is interpreted as a sign-reversing operation (Palistrant & Zamorzaev, 1964; Zamorzaev, 1976). Symbols and numbering for the 31 types of magnetic frieze groups are as follows: the symbols and numbering of the seven magnetic frieze-group types of the form **G** are given in Table 1. The numbering is given as *N*.0, where *N* denotes a sequential numbering from one to seven. The symbols for the 7 magnetic frieze-group types of the form **G1′** are the symbols for the group **G** followed by **1′**. Their numbering is *N*.1. The 17 magnetic frieze-group types of the form **G[H]** are surveyed in Table 2. The numbering of these types, given in the first column, is *N.M*, where *M* is a sequential numbering starting with 2. Symbols for these types of group are given in the second and third columns of Table 2. One symbol is that of **G[H]** and the other a primed symbol based on the symbol for **G**.

The same symbols for magnetic frieze-group types are also used as symbols for the representative group from each type. These groups are defined by their translational subgroup p or $p' = \langle(E|1,0)'\rangle$ and the coset representatives listed in Tables 1 and 2. A prime denotes multiplication with 1′.

The maximal subgroups of the magnetic frieze groups are given in Table 3. In the first column is given a numbering to each magnetic frieze group that corresponds to the numbering of the corresponding magnetic frieze-group types. The *N* in the numbering *N.M* of these 31 groups denotes the reduced magnetic superfamily to which the group belongs. This is followed by

Table 1. *The seven frieze-group types and their representative groups*

Type	Coset representatives			
1.0 $p1$	$(E\|0,0)$			
2.0 $p2$	$(E\|0,0)$	$(2\|0,0)$		
3.0 $p1m1$	$(E\|0,0)$	$(m_x\|0,0)$		
4.0 $p11m$	$(E\|0,0)$	$(m_y\|0,0)$		
5.0 $p11g$	$(E\|0,0)$	$(m_y\|\frac{1}{2},0)$		
6.0 $p2mm$	$(E\|0,0)$	$(2\|0,0)$	$(m_x\|0,0)$	$(m_y\|0,0)$
7.0 $p2mg$	$(E\|0,0)$	$(2\|0,0)$	$(m_x\|\frac{1}{2},0)$	$(m_y\|\frac{1}{2},0)$

Table 2. *The 17 magnetic frieze-group types of the form* **G[H]** *and their representative groups*

Type		Coset representatives			
1.2 $p'1$	$p1[p_21]$	$(E\|0,0)$			
2.2 $p2'$	$p2[p1]$	$(E\|0,0)$	$(2\|0,0)'$		
2.3 $p'2$	$p2[p_22]$	$(E\|0,0)$	$(2\|0,0)$		
3.2 $p1m'1$	$p1m1[p1]$	$(E\|0,0)$	$(m_x\|0,0)'$		
3.3 $p'1m1$	$p1m1[p_21m1]$	$(E\|0,0)$	$(m_x\|0,0)$		
4.2 $p11m'$	$p11m[p1]$	$(E\|0,0)$	$(m_y\|0,0)'$		
4.3 $p'11m$	$p11m[p_211m]$	$(E\|0,0)$	$(m_y\|0,0)$		
4.4 $p'11m'$	$p11m[p_211g]$	$(E\|0,0)$	$(m_y\|0,0)'$		
5.2 $p11g'$	$p11g[p1]$	$(E\|0,0)$	$(m_y\|\frac{1}{2},0)'$		
6.2 $p2'mm'$	$p2mm[p1m1]$	$(E\|0,0)$	$(2\|0,0)'$	$(m_x\|0,0)$	$(m_y\|0,0)'$
6.3 $p2'm'm$	$p2mm[p11m]$	$(E\|0,0)$	$(2\|0,0)'$	$(m_x\|0,0)'$	$(m_y\|0,0)$
6.4 $p2m'm'$	$p2mm[p2]$	$(E\|0,0)$	$(2\|0,0)$	$(m_x\|0,0)'$	$(m_y\|0,0)'$
6.5 $p'2mm$	$p2mm[p_2mm]$	$(E\|0,0)$	$(2\|0,0)$	$(m_x\|0,0)$	$(m_y\|0,0)$
6.6 $p'2m'm'$	$p2mm[p_22mg]$	$(E\|0,0)$	$(2\|0,0)$	$(m_x\|0,0)'$	$(m_y\|0,0)'$
7.2 $p2'm'g$	$p2mg[p11g]$	$(E\|0,0)$	$(2\|0,0)'$	$(m_x\|\frac{1}{2},0)'$	$(m_y\|\frac{1}{2},0)$
7.3 $p2'mg'$	$p2mg[p1m1]$	$(E\|0,0)$	$(2\|0,0)'$	$(m_x\|\frac{1}{2},0)$	$(m_y\|\frac{1}{2},0)'$
7.4 $p2m'g'$	$p2mg[p2]$	$(E\|0,0)$	$(2\|0,0)$	$(m_x\|\frac{1}{2},0)'$	$(m_y\|\frac{1}{2},0)'$

the magnetic frieze-group symbol. The remainder of the table consists of three columns containing, respectively, all type I maximal subgroups, all type II*b* maximal sub-groups and all type II*c* maximal subgroups of lowest index. For magnetic frieze groups, there are no maximal subgroups of type II*a*.

Maximal subgroups of the group $\mathbf{G} = p2$: this group has a single type I equi-translational maximal subgroup, the subgroup of index 2, $p1$. There are two type II*c* isotypic of index 2 maximal subgroups both belonging to the same magnetic frieze-group type $p2$. These two groups have translational subgroups $p_2 = \langle(E|2,0)\rangle$ and sets of coset representatives $(E|0,0)$ $(2|0,0)$, and $(E|0,0)$ $(2|1,0)$, respectively. The first is the subgroup p_22, see Table 1. The second is not an identical subgroup and a symbol must be introduced to distinguish this subgroup from the first. On moving the origin of the coordinate system in which the group $\mathbf{G} = p2$ is defined to $(\frac{1}{2},0)$, this second group is defined by the translational subgroup p_2 and the coset representatives $(E|0,0)$ $(2|0,0)$. Consequently, we denote this second subgroup as p_22 $(\frac{1}{2},0)$.

Maximal subgroups of the group $\mathbf{G1}' = p21'$: $\mathbf{G} = p2$ is a type I maximal subgroup of index 2. There are three maximal subgroups of $\mathbf{G} = p2$, *i.e.* $p1$, p_22 and p_22 $(\frac{1}{2},0)$. Consequently, $\mathbf{G1}' = p21'$ has three additional maximal subgroups $p11'$, p_221' and p_221' $(\frac{1}{2},0)$. There are three subgroups of index 2 of $\mathbf{G} = p2$, *i.e.* $p1$, p_22 and $p_22(\frac{1}{2},0)$. Consequently, $\mathbf{G1}' = p21'$ has three additional maximal subgroups $p2[p1] = p2'$, $p2[p_22] = p'2$ and $p2[p_22(\frac{1}{2},0)] = p'2(\frac{1}{2},0)$. These are the seven maximal subgroups of $\mathbf{G1}' = p21'$ listed in Table 3.

Maximal subgroups of $\mathbf{G[H]} = p2[p_22] \equiv p'2$: $\mathbf{H} = p_22$ is a maximal subgroup of index 2. The maximal subgroups of $\mathbf{G} \neq \mathbf{H}$ listed in Table 3 are $\mathbf{S}_G = p1$ and $p_22(\frac{1}{2},0)$. The only subgroup of index 2 of $\mathbf{S}_G$ that is contained in $\mathbf{H}$ is $\mathbf{K} = p_21$. Consequently, $\mathbf{S}_G[\mathbf{K}] = p1[p_21] \equiv p'1$ and $p_22(\frac{1}{2},0)[p_21] = p_22'(\frac{1}{2},0)$ are maximal subgroups of $p'2$. We have not found as yet the type II*c* maximal subgroups of lowest index. This is because we have considered only the maximal subgroups of $\mathbf{G} = p2$ listed in Table 3 where only the type II*c* maximal subgroups of lowest index are given. The next-lowest type II*c* maximal subgroups of $\mathbf{G} = p2$ are the index 3 subgroups p_32, p_32 $(1,0)$ and p_32 $(2,0)$. Each of these contain two subgroups of index 2, *e.g.* for $\mathbf{S}_G = p_32$ the two subgroups are p_31 and p_62, only the latter of which is a subgroup of $\mathbf{H} = p_22$. Consequently, $\mathbf{S}_G[K] = p_32[p_62] \equiv p'_32$ is a maximal subgroup. There are then three type II*c* maximal subgroups of lowest index of $\mathbf{G[H]} = p2[p_22] \equiv p'2$, the three groups p'_32, p'_32 $(1,0)$ and p'_32 $(2,0)$.

This work was supported by the National Science Foundation under grant DMR-9510335.

APPENDIX A
Proof of procedure

(*A*1) *To find the maximal subgroups of* **G1**′. There are three forms of subgroups of **G1**′: (*a*) **P** where $\mathbf{P} \subseteq \mathbf{G}$; (*b*) **P1**′ where $\mathbf{P} \subset \mathbf{G}$; (*c*) **P[H]** where $\mathbf{P} \subseteq \mathbf{G}$.

(*A*1*a*) $\mathbf{P} = \mathbf{G}$ is a subgroup of index 2 of **G1**′ and therefore a maximal subgroup of **G1**′. If $\mathbf{P} \subset \mathbf{G}$, then **P** is not a maximal subgroup of **G1**′ since it is a subgroup of the maximal subgroup **G**.

(*A*1*b*) $\mathbf{P1}' = \mathbf{S}_G\mathbf{1}'$, where $\mathbf{S}_G$ is a maximal subgroup of **G**, as it contains the element 1′, is not a subgroup of subgroups of the form **P** or **P[H]**. It is not a subgroup of some other group **P1**′ as that would imply that $\mathbf{S}_G$ is not a maximal subgroup of **G**. Consequently, $\mathbf{S}_G\mathbf{1}'$ is a maximal subgroup. Any subgroup **P1**′ where $\mathbf{P} \subset \mathbf{S}_G$ is not maximal since $\mathbf{P1}' \subset \mathbf{S}_G\mathbf{1}'$.

(*A*1*c*) If $\mathbf{P} \subset \mathbf{G}$ then $\mathbf{P[H]} \subset \mathbf{P1}'$, and only if $\mathbf{P} = \mathbf{G}$ can **P[H]** be a maximal subgroup. Every **G[H]** is a subgroup of index 2 of **G1**′ and consequently every **G[H]** is a maximal subgroup.

(*A*2) *To find maximal subgroups of* **G[H]**. There are two forms of subgroups of **G[H]**: (*a*) **P** where $\mathbf{P} \subseteq \mathbf{H}$, (*b*) **P[K]** where $\mathbf{P} \subset \mathbf{G}$, $\mathbf{P} \not\supseteq \mathbf{H}$ and $\mathbf{K} \subset \mathbf{H}$.

(*A*2*a*) $\mathbf{P} = \mathbf{H}$ is a subgroup of index 2 and therefore maximal. Any subgroup $\mathbf{P} \subset \mathbf{H}$ is then not a maximal subgroup of **G[H]**.

Table 3. *Maximal subgroups of the magnetic frieze groups*

Type I		Type IIb		Type IIc	
1.0 *p*1					
				[2] $p_{2}1$	
1.1 *p*11′					
[2] *p*1		[2] *p*′1		[2] $p_{2}11'$	
1.2 *p*′1 ≡ *p*1[$p_{2}1$]					
		[2] $p_{2}1$		[3] $p'_{3}1$	
2.0 *p*2					
[2] *p*1				[2] $p_{2}2$	
				[2] $p_{2}2$	(½, 0)
2.1 *p*21′					
[2] *p*2		[2] *p*′2		[2] $p_{2}21'$	
[2] *p*11′		[2] *p*′2	(½, 0)	[2] $p_{2}21'$	(½, 0)
[2] *p*2′					
2.2 *p*2′ ≡ *p*2[*p*1]					
[2] *p*1				[2] $p_{2}2'$	
				[2] $p_{2}2'$	(½, 0)
2.3 *p*′2 ≡ *p*2[$p_{2}2$]					
[2] *p*′1		[2] $p_{2}2$		[3] $p'_{3}2$	
		[2] $p_{2}2'$	(½, 0)	[3] $p'_{3}2$	(1, 0)
				[3] $p'_{3}2$	(2, 0)
3.0 *p*1*m*1					
[2] *p*1				[2] $p_{2}1m1$	
				[2] $p_{2}1m1$	(½, 0)
3.1 *p*1*m*11′					
[2] *p*1*m*1		[2] *p*′1*m*1		[2] $p_{2}1m11'$	
[2] *p*11′		[2] *p*′1*m*1	(½, 0)	[2] $p_{2}1m11'$	(½, 0)
[2] *p*1*m*′1					
3.2 *p*1*m*′1 ≡ *p*1*m*1[*p*1]					
[2] *p*1				[2] $p_{2}1m'1$	
				[2] $p_{2}1m'1$	(½, 0)
3.3 *p*′1*m*1 ≡ *p*1*m*1[$p_{2}1m1$]					
[2] *p*′1		[2] $p_{2}1m1$		[3] $p'_{3}1m1$	
		[2] $p_{2}1m'1$	(½, 0)	[3] $p'_{3}1m1$	(1, 0)
				[3] $p'_{3}1m1$	(2, 0)
4.0 *p*11*m*					
[2] *p*1		[2] $p_{2}11g$		[2] $p_{2}11m$	
4.1 *p*11*m*1′					
[2] *p*11*m*		[2] $p_{2}11g1'$		[2] $p_{2}11m1'$	
[2] *p*11′		[2] *p*′11*m*′			
[2] *p*11*m*′		[2] *p*′11*m*			
4.2 *p*11*m*′ ≡ *p*11*m*[*p*1]					
[2] *p*1		[2] $p_{2}11g'$		[2] $p_{2}11m'$	
4.3 *p*′11*m* ≡ *p*11*m*[$p_{2}11m$]					
[2] *p*′1		[2] $p_{2}11m$		[3] $p'_{3}11m$	
		[2] $p_{2}11g'$			
4.4 *p*′11*m*′ ≡ *p*11*m*[$p_{2}11g$]					
[2] *p*′1		[2] $p_{2}11g$		[3] $p'_{3}11m'$	
		[2] $p_{2}11m'$			
5.0 *p*11*g*					
[2] *p*1				[3] $p_{3}11g$	
5.1 *p*11*g*1′					
[2] *p*11*g*				[3] $p_{3}11g1'$	
[2] *p*11′					
[2] *p*11*g*′					
5.2 *p*11*g*′ ≡ *p*11*g*[*p*1]					
[2] *p*1				[3] $p_{3}11g'$	
6.0 *p*2*mm*					
[2] *p*2		[2] $p_{2}2mg$		[2] $p_{2}2mm$	
[2] *p*1*m*1		[2] $p_{2}2mg$	(½, 0)	[2] $p_{2}2mm$	(½, 0)
[2] *p*11*m*					
6.1 *p*2*mm*1′					
[2] *p*2*mm*		[2] *p*′2*m*′*m*′		[2] $p_{2}2mm1'$	
[2] *p*21′		[2] *p*′2*m*′*m*′	(½, 0)	[2] $p_{2}2mm1'$	(½, 0)
[2] *p*1*m*11′		[2] *p*′2*mm*			

Table 3 (*cont.*)

Type I		Type IIb		Type IIc	
[2] *p*11*m*1′		[2] *p*′2*mm*	(½, 0)		
[2] *p*2*m*′*m*′		[2] $p_{2}2mg1'$			
[2] *p*2′*mm*′		[2] $p_{2}2mg1'$	(½, 0)		
[2] *p*2′*m*′*m*					
6.2 *p*2′*mm*′ ≡ *p*2*mm*[*p*1*m*1]					
[2] *p*1*m*1		[2] $p_{2}2'mg'$		[2] $p_{2}2'mm'$	
[2] *p*2′		[2] $p_{2}2'mg'$	(½, 0)	[2] $p_{2}2'mm'$	(½, 0)
[2] *p*11*m*′					
6.3 *p*2′*m*′*m* ≡ *p*2*mm*[*p*11*m*]					
[2] *p*11*m*		[2] $p_{2}2'm'g$		[2] $p_{2}2'm'm$	
[2] *p*1*m*′1		[2] $p_{2}2'm'g$	(½, 0)	[2] $p_{2}2'm'm$	(½, 0)
[2] *p*2′					
6.4 *p*2*m*′*m*′ ≡ *p*2*mm*[*p*2]					
[2] *p*2		[2] $p_{2}2m'g'$		[2] $p_{2}2m'm'$	
[2] *p*1*m*′1		[2] $p_{2}2m'g'$	(½, 0)	[2] $p_{2}2m'm'$	(½, 0)
[2] *p*11*m*′					
6.5 *p*′2*mm* ≡ *p*2*mm*[$p_{2}2mm$]					
[2] *p*′2		[2] $p_{2}2mm$		[3] $p'_{3}2mm$	
[2] *p*′1*m*1		[2] $p_{2}2m'g'$		[3] $p'_{3}2mm$	(1, 0)
[2] *p*′11*m*		[2] $p_{2}2'mg'$	(½, 0)	[3] $p'_{3}2mm$	(2, 0)
		[2] $p_{2}2'm'm$	(½, 0)		
6.6 *p*′2*m*′*m*′ ≡ *p*2*mm*[$p_{2}2mg$]					
[2] *p*′2		[2] $p_{2}2mg$		[3] $p'_{3}2m'm'$	
[2] *p*′1*m*1	(½, 0)	[2] $p_{2}2'm'g$	(½, 0)	[3] $p'_{3}2m'm'$	(1, 0)
[2] *p*′11*m*′		[2] $p_{2}2m'm'$		[3] $p'_{3}2m'm'$	(2, 0)
		[2] $p_{2}2'mm'$	(½, 0)		
7.0 *p*2*mg*					
[2] *p*2				[3] $p_{3}2mg$	
[2] *p*1*m*1	(¼, 0)			[3] $p_{3}2mg$	(1, 0)
[2] *p*11*g*				[3] $p_{3}2mg$	(2, 0)
7.1 *p*2*mg*1′					
[2] *p*2*mg*				[3] $p_{3}2mg1'$	
[2] *p*21′				[3] $p_{3}2mg1'$	(1, 0)
[2] *p*1*m*11′	(¼, 0)			[3] $p_{3}2mg1'$	(2, 0)
[2] *p*11*g*1′					
[2] *p*2*m*′*g*′					
[2] *p*2′*mg*′					
[2] *p*2′*m*′*g*					
7.2 *p*2′*m*′*g* ≡ *p*2*mg*[*p*11*g*]					
[2] *p*11*g*				[3] $p_{3}2'm'g$	
[2] *p*2′				[3] $p_{3}2'm'g$	(1, 0)
[2] *p*1*m*′1	(¼, 0)			[3] $p_{3}2'm'g$	(2, 0)
7.3 *p*2′*mg*′ ≡ *p*2*mg*[*p*1*m*1]					
[2] *p*1*m*1	(¼, 0)			[3] $p_{3}2'mg'$	
[2] *p*2′				[3] $p_{3}2'mg'$	(1, 0)
[2] *p*11*g*′				[3] $p_{3}2'mg'$	(2, 0)
7.4 *p*2*m*′*g*′ ≡ *p*2*mg*[*p*2]					
[2] *p*2				[3] $p_{3}2m'g'$	
[2] *p*1*m*′1	(¼, 0)			[3] $p_{3}2m'g'$	(1, 0)
[2] *p*11*g*′				[3] $p_{3}2m'g'$	(2, 0)

(*A2b*) If $\mathbf{P} = \mathbf{S}_G \neq \mathbf{H}$ then $\mathbf{S}_G[\mathbf{K}]$ is a maximal subgroup. If not, this would imply the existance of a subgroup $\mathbf{P}[\mathbf{Q}]$ such that $\mathbf{S}_G[\mathbf{K}] \subset \mathbf{P}[\mathbf{Q}] \subset \mathbf{G}[\mathbf{H}]$, where $\mathbf{S}_G \subset \mathbf{P} \subset \mathbf{G}$, which contradicts the assumption that $\mathbf{S}_G$ is a maximal subgroup of $\mathbf{G}$. If $\mathbf{P} \subset \mathbf{S}_G$ then $\mathbf{P}[\mathbf{K}]$ is not a maximal subgroup of $\mathbf{G}[\mathbf{H}]$. If $\mathbf{P} \subset \mathbf{S}_G$ then we can show that there exists a subgroup $\mathbf{S}_G[\mathbf{Q}]$ of $\mathbf{G}[\mathbf{H}]$ such that $\mathbf{P}[\mathbf{K}] \subset \mathbf{S}_G[\mathbf{Q}] \subset \mathbf{G}[\mathbf{H}]$. We can write $\mathbf{P}[\mathbf{K}] = \mathbf{K} + g'\mathbf{K}$ where $g \in \mathbf{G} - \mathbf{H}$ and $\mathbf{P} = \mathbf{K} + g\mathbf{K}$. We can also write $\mathbf{G}[\mathbf{H}] = \mathbf{H} + g'\mathbf{H}$ with the same element $g \in \mathbf{G} - \mathbf{H}$ and $\mathbf{G} = \mathbf{H} + g\mathbf{H}$. Since $\mathbf{P} \subset \mathbf{S}_G$,

$$S_G = P + a_2P + \ldots . + a_NP$$

and

$$S_G = (K + gK) + a_2(K + gK) + \ldots . + a_N(K + gK),$$

where each element $a_i = h_i \in \mathbf{H}$ or $a_i = gh_i \in g\mathbf{H}$. Since $\mathbf{G} = \mathbf{H} + g\mathbf{H}$, if $a_i = h_i$ then $h_i(\mathbf{K} + g\mathbf{K}) = h_i\mathbf{K} + h_i g\mathbf{K}$, where $h_i\mathbf{K} \in \mathbf{H}$ and $h_i g\mathbf{K} \in g\mathbf{H}$, and if $a_i = gh_i$ then $gh_i(\mathbf{K} + g\mathbf{K}) = gh_i\mathbf{K} + gh_i g\mathbf{K}$, where $gh_i\mathbf{K} \in g\mathbf{H}$ and $gh_i g\mathbf{K} \in \mathbf{H}$. Consequently, half the elements of $\mathbf{S}_G$ are in $\mathbf{H}$ and half are in $\mathbf{G} - \mathbf{H} = g\mathbf{H}$. This subset Q of elements in $\mathbf{S}_G$ which are in $\mathbf{H}$ constitutes a subgroup $\mathbf{Q}$ of index 2 of $\mathbf{S}_G$: (i) since the elements of the group $\mathbf{K}$ are contained in Q, Q contains an identity; (ii) since $\mathbf{S}_G$ is a group, $h_ih_j \in \mathbf{S}_G$. Since $\mathbf{H}$ is a group, $h_ih_j \in \mathbf{H}$. Therefore, $h_ih_j \in Q$; (iii) each element h of Q has an inverse s_G in $\mathbf{S}_G$, $hs_G = e$, where the identity e is contained in Q. $s_G = h_j \in \mathbf{H}$ or $s_G = gh_j \in g\mathbf{H}$. The latter case is not possible since $hgh_j \in g\mathbf{H}$, which does not contain the identity element. We have then that the inverse of every element in the set Q is also in this set. Consequently, the elements of the set Q constitute a subgroup of $\mathbf{Q}$ index 2 of $\mathbf{S}_G$. Finally, $\mathbf{S}_G[\mathbf{Q}]$ is a subgroup of $\mathbf{G}[\mathbf{H}]$ such that $\mathbf{P}[\mathbf{K}] \subset \mathbf{S}_G[\mathbf{Q}] \subset \mathbf{G}[\mathbf{H}]$.

References

Belov, N. V. (1956). *Sov. Phys. Crystallogr.* **1**, 372–374.

Bieberbach, I. (1912). *Math. Ann.* **72**, 400–412.

Billiet, Y. (1981). *Acta Cryst.* **A37**, 649–652.

Cracknell, A. P. (1975). *Magnetism in Crystalline Materials.* Oxford/New York: Pergamon.

Hermann, C. (1929). *Z. Kristallogr.* **69**, 533–555.

International Tables for Crystallography (1983). Vol. A, edited by Th. Hahn. Dordrecht: Kluwer Academic Publishers. [Revised editions 1987, 1989 and 1995.]

Litvin, D. B. (1996). In preparation.

Opechowski, W. (1986). *Crystallographic and Metacrystallographic Groups.* Amsterdam: North Holland.

Palistrant, A. F. & Zamorzaev, A. M. (1964). *Sov. Phys. Crystallogr.* **9**, 123–128.

Zamorzaev, A. M. (1976). *The Theory of Simple and Multiple Antisymmetry.* Kishinev: Shtiintsa. (In Russian.)