Magnetic Group Tables

1-, 2- and 3-Dimensional Magnetic Subperiodic Groups and Magnetic Space Groups

Part 1. Introduction

Daniel B. Litvin



Magnetic Group Tables

%lž&l[·]UbX[·]' !8]a Ybg]cbU[·]AU[bYh]WGiVdYf]cX]W;fcidg UbX[·]AU[bYh]WGdUWY[·];fcidg

Part 1. Introduction

Daniel B. Litvin Department of Physics the Eberly College of Science The Pennsylvania State University Penn State Berks

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ISBN 978-0-9553602-2-0 doi:10.1107/9780955360220001 Reviewed by the IUCr Commission on Magnetic Structures To my family:

To Tikva Sa'eeda

יזכרונה לברכה - may her memory be a blessing

green-eyed and raven-haired, how wonderful life was while she was in this world. אוהב אותך ומתגעגע

To Usa Shoshana and Steven Yitzchak

our kids who have always done us proud.

and

To Talia Sa'eeda Aiko

the most beautiful granddaughter in the whole wide world. mach mach from Babajoon.

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Preface

Preface

This work tabulates the structure, symbols, and properties of magnetic groups. A survey of magnetic group types is presented listing the elements of one representative group of the 5, 31, and 122 types of groups in, respectively, the reduced superfamilies of the 1-, 2-, and 3-dimensional magnetic point groups, the 31, 394, and 528 types of groups in, respectively, the reduced superfamilies of magnetic subperiodic groups, i.e. magnetic frieze groups, magnetic rod groups , and mgnetic layer groups, and the 7, 80, and 1651 types of groups in, respectively, the reduced superfamilies of 1-, 2-, and 3-dimensional magnetic space groups. Tables of properties of the 1-, 2-, and 3-dimensional magnetic subperiodic and magnetic space groups are given, an extension of the classic work in the *International Tables for Crystallography, Volume A: Space Group Symmetry* and the *International Tables for Crystallography, Volume E: Subperiodic Groups.* We then compare Opechowski-Guccione and Belov-Nerenova-Smirnova magnetic group symbols, and list maximal subgroups of index < 4.

Previous versions of parts of this work were published over the past decade with the financial support of the National Science Foundation under grants DMR-9722799 and DMR-0074550. This work has undergone substantial revisions as it was not computer generated, but hand calculated and typed, and consequently the probability for errors and/or typos was then not zero. Two years of rechecking has decreased substantially the number of these errors and/or typos, but realistically not to zero. The exception is thanks to Drs. H. Stokes and B. Campbell of Brigham Young University who parsed and computer checked the survey of 3-dimensional magnetic space groups .

Preface

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November 2022: All errors and typos known to this date have been corrected.

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The *subperiodic groups* in the title refer to the crystallographic frieze groups, 2dimensional groups with 1-dimensional translations, crystallographic rod groups, 3dimensional groups with 1-dimensional translations, and crystallographic layer groups, 3-dimensional groups with 2-dimensional translations. There are 7 frieze group types ¹, 75 rod group types ²⁻⁵, and 80 layer group types ^{2, 5-12} (also see *Vol. E: Subperiodic Groups* of the *International Tables for Crystallography* ¹³ [abbreviate as *ITC-E*] and Shubnikov and Koptsik ¹⁴). The *space groups* in the title refer to the 1-, 2-, and 3dimensional crystallographic space groups, n-dimensional groups with n-dimensional translations. There are 2 1-dimensional space group types ¹⁵⁻¹⁷ (also see *Vol. A: Space Groups* of the *International Tables for Crystallography* ¹⁸ [abbreviate as *ITC-A*] and Burns and Glazer ¹⁹).

Magnetic groups are symmetry groups of spin arrangements and were introduced by Landau and Lifschitz^{20, 21} by reinterpreting the operation of "change in color" in 2-color (black and white, antisymmetry) crystallographic groups as "time inversion." The crystallographic 2-color point group types had been given by Heesch²² and Shubnikov²³. 2-color subperiodic groups consist of 31 2-color frieze group types²⁴, 394 2-color rod group types²⁵⁻²⁷, and 528 2-color layer group types^{25,28}. There are 7 2color one-dimensional space group types²⁵, 80 2-color two-dimensional space group types^{9,29}, and 1651 2-color three-dimensional space group types³⁰⁻³² (also see Zamorzaev³³, Koptsik³⁴, and Zamorzaev and Palistrant³⁵).

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The 3-dimensional magnetic space groups were rederived by Opechowski and Guccione ^{36,37} using a methodology different from that used by Belov, Neronova, and Smirnova ³² in deriving 2-color 3-dimensional space groups. This has led to a difference in symbols used to denote the magnetic group types (See Section 3). The 1-, 2-, and 3-dimensional magnetic subperiodic and 1- and 2-dimensional space groups have also been re-derived ³⁸⁻⁴¹. The group type symbols used are based on the symbols for the subperiodic group types ¹³ and space group types ¹⁸ and constructed in analogy to the Opechowski and Guccione ^{36,37,42} symbols for the 3-dimensional magnetic space group types.

In Section 1: Survey of Magnetic Groups, a survey of 1-, 2-, and 3-dimensional magnetic point groups, magnetic subperiodic groups, and magnetic space groups is given emphasizing their mathematical structure and classification into *reduced magnetic superfamilies* ³⁷ of groups. In Section 2: Tables of Properties of Magnetic Groups, we present tables of crystallographic properties of the 1-, 2-, and 3-dimensional magnetic subperiodic groups and magnetic space groups. The material is similar in content and format to the crystallographic properties of the subperiodic groups found in *ITC-E* ¹³ and of space groups found in *ITC-A* ¹⁸. In Section 3: OG/BNS Magnetic Group Type Symbols, the symbols for magnetic group types constructed in analogy to Opechowski and Guccione ^{36,37} symbols of 3-dimensional magnetic space group types are compared with symbols of 2-color group types constructed in analogy to Belov, Neronova, and Smirnova ³² symbols for 2-color 3-dimensional space group types. In

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Section 4: Maximal Subgroups of Index \leq 4, we give the maximal subgroups of index \leq 4 of the representative groups of the 1-, 2-, and 3-dimensional magnetic subperiodic group types and magnetic space group types.

Section 1: Survey of Magnetic Groups

In Section 1.1 we review the concept of *reduced magnetic superfamily* ³⁷ to provide a classification scheme for magnetic groups. This is used in Section 1.2 to obtain a survey of 1-, 2-, and 3-dimensional magnetic point groups types, magnetic subperiodic group types and magnetic space group types. In this survey we provide a specification of a single *representative group* from each group type.

1.1 Reduced magnetic superfamily of magnetic groups

Let F denote a crystallographic group. The *magnetic superfamily* of F consists of ³⁷ :

- 1) The group F.
- 2) The group F1' ≡ F × 1', the direct product of the group F and the time inversion group 1', the latter consisting of the identity 1 and time inversion 1'.
- All groups F(D) = D + (F D)1' = F ≚ 1', subdirect products of the groups F and 1'. D is a subgroup of index two of F. Groups of this kind will also be denoted by M.

For magnetic space groups and magnetic subperiodic groups, this third set of groups is divided into two subdivisions:

- 3a) Groups M_{τ} , where D is an equi-translational subgroup of F.
- 3b) Groups M_R , where D is an equi-class subgroups of F. Groups M_R can be written as $M_R = D + t_{\alpha}' D$ where t_{α} is a translation contained in F but not in

D. The choice of t_{α} is not unique, but can be exchanged with any other translation contained in F but not in D. In these tables, the choice of t_{α} is given in Tables 1.1 ^{36,41}.

If only non-equivalent ³⁷ groups F(D) are included, then the above set of groups is referred to as the *reduced magnetic superfamily* of F.

As an example we consider the crystallographic point group $F = 2_x 2_y 2_z$. The magnetic superfamily of the group $2_x 2_y 2_z$ consists of the five groups: $F = 2_x 2_y 2_z$; the group $F1' = 2_x 2_y 2_z 1'$, and the three groups $F(D) = 2_x 2_y 2_z (2_x)$, $2_x 2_y 2_z (2_y)$, and $2_x 2_y 2_z (2_z)$. Since the latter three groups are all equivalent, the reduced magnetic superfamily of the group $2_x 2_y 2_z$ consists of only three groups, $2_x 2_y 2_z$, $2_x 2_y 2_z 1'$, and one of the three groups $2_x 2_y 2_z (2_x)$, $2_x 2_y 2_z (2_y)$, and $2_x 2_y 2_z (2_z)$.

A magnetic group has been defined as a symmetry group of a spin arrangement $S(r)^{37}$. With this definition, since 1'S(r) = -S(r), a group F1' is then not a magnetic group, in the sense that it can never be an invariance group of a magnetic structure with non-zero spins. However there is not universal agreement on the definition or usage of the term *magnetic group*. Two definitions³⁷ have magnetic groups as symmetry groups of spin arrangements, with one having only groups F(D) defined as magnetic groups. Here we shall refer to magnetic groups as all groups in a magnetic superfamily of a group F, while cognizant of the fact that groups F1' can not be a symmetry group of a spin arrangement. We shall at times refer to a group which as no element coupled with time inversion 1', as the group D in the magnetic group F(D), as a non-primed group.

1.2 Survey of 1-, 2-, and 3-dimensional magnetic point groups, magnetic subperiodic groups, and magnetic space groups

The survey here consists of listing the reduced magnetic superfamily of one group from each type of 1-, 2-, and 3-dimensional crystallographic point group, listing the reduced magnetic superfamily of one group from each type of 1-, 2-, and 3dimensional subperiodic group, and listing the reduced magnetic superfamily of one group from each type of 1-, 2-, and 3-dimensional space group. The number of types of groups F, F1', and F(D) in the reduced magnetic superfamilies of 1-, 2-, 3dimensional crystallographic point groups, subperiodic groups and space groups is given in Figure 1.2.1. For magnetic subperiodic and magnetic space groups we also give the subdivision of the number of F(D) group types into M_{T} and M_{R} type groups.

2-, and 3-dimensional crystallographic point groups, subperiodic groups and space groups.						
		F	F1'	F(D)	Total	
1-Dimensional Ma Point G	agnetic Groups	2	2	1	5	
2-Dimensional Ma Point G	agnetic Groups	10	10	11	31	
3-Dimensional Ma Point G	agnetic Groups	32	32	58	122	

Figure 1.2.1. Number of types of groups in the reduced magnetic superfamilies of 1-,

	F	F1'	F(D)) [M _T	M _R]	Total
Magnetic Frieze Groups	7	7	17	[10	7]	31
Magnetic Rod Groups	75	75	244	[169	75]	394
Magnetic Layer Groups	80	80	368	[246	122]	528
1-Dimensional Magnetic Space Groups	2	2	3	[1	2]	7
2-Dimensional Magnetic Space Groups	17	17	46	[26	20]	80
3-Dimensional Magnetic Space Groups	230	230	1191	[674	517]	1651

The one group from each type, called the *representative group* of that type, is specified by listing, for magnetic point groups, the elements of the representative group, and for magnetic space groups and magnetic subperiodic groups, a set of coset representatives, called the *standard set of coset representatives*, of the decomposition of the group with respect to its translational subgroup.

The survey is given in The Survey of Magnetic Group Types in The Magnetic

Group Tables. The information provided for each group type is:

1) The serial number of the magnetic group type.

2) The symbol of the magnetic group type which serves also as the symbol of the group type's representative group.

3) For magnetic point groups, the elements of the representative group. For magnetic space groups and magnetic subperiodic groups, a standard set of coset

representatives of the decomposition of the representative group with respect to its translational subgroup.

4) For group types F(D): The symbol of the group type of the non-primed subgroup D of index two of the representative group F(D) is given. The orientation (for magnetic point groups) or origin and orientation (for magnetic space groups and magnetic subperiodic groups) is also given of a new coordinate system for the nonprimed subgroup D in the coordinate system of the representative group F. In this new coordinate system, the group D is identical with the representative group of D given in the tables.

Examples of the format of *The Survey of Magnetic Group Types* from *The Magnetic*

Group Tables are given in Figure 1.2.2.

Dimensional Magnetic Space Group Types and 3-Dimensional Magnetic Point Group Types from *The Magnetic Group Tables*: Serial Non-primed Subgroup Number of Index Two Standard Set of Coset Representatives Symbol 10.3.51 P2'/m Pm (1|0,0,0) $(2_{v}|0,0,0)'$ (1|0,0,0)' (m_v|0,0,0) (0,0,0;a,b,c) 10.9.57 $P_{2h}2'/m$ $P2_1/m$ (0, $\frac{1}{2}$,0;a,2b,c) (1|0,0,0) $(2_v | 0, 1, 0)$ ($\overline{1} | 0, 1, 0$) $(m_{v}|0,0,0)$ 50.10.386 P_{2c}b'a'n' Pnnn $(\frac{1}{4}, \frac{1}{4}, \frac{1}{2}; a, 2\overline{c}, b)$ (1|0,0,0) $(2_x|0,0,0)$ $(2_y|0,0,1)$ $(2_z|0,0,1)$ $(\overline{1}|_{2}, \overline{2}, 1)$ $(m_x|_{2}, \overline{2}, 1)$ $(m_y|_{2}, \overline{2}, 0)$ $(m_z|_{2}, \overline{2}, 0)$ Serial Non-primed Subgroup Number Symbol of Index Two Representative Point Group 8.3.26 mm2 2_x m_x' 2,' 2_z' m'mm (b,c,a) 1 1' ḿ, m, 2_y' m_v' 2_z 8.4.27 2,' m'm'm 2/m (a,b,c) 1 1 mĴ.' m,

Figure 1.2.2: Examples of format of The Survey of Magnetic Group Types of 3-

1.2.1 Magnetic group type serial number

For each set of magnetic group types, 1-, 2-, and 3-dimensional crystallographic magnetic point groups, magnetic subperiodic groups, and magnetic space groups, a separate numbering system is used. A three part composite number $N_1.N_2.N_3$ is given in the first column, see Figure 1.2.2. N_1 is a sequential number for the group type to which F belongs. N_2 is a sequential numbering of the magnetic group types of the reduced magnetic superfamily of F. Group types F always have the assigned number $N_1.1.N_3$, and group types F1' the assigned number $N_1.2.N_3$. N_3 is a global sequential numbering for each set of magnetic group types. The sequential numbering N_1 for subperiodic groups and space groups follows the numbering in the *ITC-E*¹³ and *ITC-A*¹⁸, respectfully.

1.2.2 Magnetic group type symbol

A Hermann-Mauguin type symbol is given for each magnetic group type in the second column. This symbol denotes both the group type and the representative group of that type. For example the symbol for the 3-dimensional magnetic space group type 25.4.158 is Pm'm'2. This symbol denotes both the group type, i.e. which consists of an infinite set of groups, and the representative group $Pm_x'm_y'2_z$. While this representative group may be referred to as "the group Pm'm'2 ", other groups of this group type, e.g. $Pm_y'm_z'2_x$, will always be written with subindicies. The representative group of the magnetic group type is defined by its translational subgroup, implied by the first letter in the magnetic group type symbol and defined in Table 1.1, and a given set of coset

representatives, called the *standard set of coset representatives*, of the representative group with respect to its translational subgroup.

Only the relative lengths and mutual orientations of the translation vectors of the translational subgroup are given, see Table 1.2. The symmetry directions of symmetry operations represented by characters in the Hermann-Mauguin symbols implied by the character's position in the symbol are given in Table 1.3. The standard set of coset representatives are given with respect to an implied coordinate system. The absolute lengths of translation vectors, the position in space of the origin of the coordinate system are not explicitly given.

1.2.3 Standard set of coset representatives

The standard set of coset representatives of each representative group of each magnetic space group type and magnetic subperiodic group type is listed on the right hand side of *The Survey of Magnetic Group Types* in *The Magnetic Group Tables*. Each coset in the standard set of coset representatives is given in Seitz notation (see Figure 1.2.2), i.e. (R| τ) or (R | τ)'. "R" denotes a proper or improper rotation (rotation-inversion), " τ " a non-primitive translation, with components denoted by τ_x , τ_y , τ_y , and the prime denotes that (R | τ) is coupled with time inversion. The subindex notation on R, denoting the orientation of the proper or improper rotation, is explained in Table 1.4.

1.2.4 Group D of groups F(D)

For magnetic group types F(D), the magnetic group type symbol of the group D is given in the third column of the survey of magnetic groups, see Figure 1.2.2. This is the magnetic group type of the subgroup D of any group of the magnetic group type F(D). It is also the symbol of the subgroup D of index 2 of the representative group F(D).

If F(D) is a group M_{τ} , then the subgroup D is defined by the translational group of F(D) and the unprimed coset representatives of F(D). For example, consider the 3dimensional magnetic space group type 16.3.101 P2'2'2. The representative group P2'2'2 is defined by the translational subgroup P generated by the translations

 $(1 | 1,0,0) \qquad (1 | 0,1,0) \qquad (1 | 0,0,1)$

and the standard set of coset representatives:

(1 | 0,0,0) $(2_x | 0,0,0)'$ $(2_y | 0,0,0)'$ $(2_z | 0,0,0)$

The subgroup D of index two of the representative group F(D) = P2'2'2 is defined by the translational group P and the cosets (1 |0,0,0) and (2_z|0,0,0), and is a group of type P2.

If F(D) is a group M_R , then the subgroup D is defined by the unprimed translational group of F(D) and all the cosets of the standard set of coset representatives of the group F(D). For example, consider the 3-dimensional magnetic space group type 16.4.102 P_{2a} 222 . The representative group P_{2a} 222 is defined by the translational group P_{2a} generated by the translations

(1 |1,0,0)' (1 |0,1,0) (1 |0,0,1)

and the standard set of coset representatives:

(1 | 0,0,0) $(2_x | 0,0,0)$ $(2_y | 0,0,0)$ $(2_z | 0,0,0).$

The subgroup D of index two of the representative group $F(D) = P_{2a}222$ is defined by

the unprimed translations of P_{2a} , i.e. the translations generated by

(1 | 2,0,0) (1 | 0,1,0) (1 | 0,0,1)

and the standard set of cosets of P_{2a} 222. The group D is a group of type P222.

While the group type symbol of D is given, the coset representatives of the subgroup D of F(D) derived from the standard set of coset representatives of F(D) may not be identical with the standard set of coset representatives of the representative group of type D found in the survey of magnetic group types. Consequently, to show the relationship between this subgroup D and the representative group of groups of type D listed in *The Magnetic Group Tables*, additional information is provided to define a second coordinate system in which the coset representatives of this subgroup D are identical with the standard set of coset representatives listed for the representative group of groups of type D.

Let (O;a,b,c) be the coordinate system in which the group F and F(D) is defined. "O" is the origin of the coordinate system, and a, b, and c are the basis vectors of the coordinate system. a, b, and c represent a set of basis vectors of a primitive cell for primitive lattices and of a conventional cell for centered lattices. The second coordinate system is defined by (O+t;a',b',c'). Here a',b',c' define the conventional unit cell of the non-primed subgroup D of the magnetic group F(D). The origin is first translated from O

to O+t, and then the basis vectors a, b, and c are changed to a', b' and c'. (On translating the origin from O to O+t, a coset representative (R | τ) becomes ^{40,41}

 $(R \mid \tau + Rt - t)$). Immediately following the group type symbol for the subgroup D of F(D) we give the second coordinate system (O+t;a',b',c') for the conventional unit cell of the group D in which the coset representatives of the subgroup D of F(D) are identical with the standard set of coset representatives of the representative group of groups of type D. In *The Magnetic Group Tables*, for typographical simplicity, the symbols "O+" are omitted. t, a', b', and c' are given in terms of the basis vectors of the coordinate system (O;a,b,c) of the group F and F(D).

Example 1: For the 3-dimensional magnetic space group type 10.4.52 P2/m', one finds in *The Magnetic Group Tables*:

Serial Number	ial Non-primed Subgroup nber Symbol of Index Two				rd Set of Cos	et Represent	atives
10.4.52	P2/m'	P2	(0,0,0;a,b,c)	(1 0,0,0)	(2 _y 0,0,0)	(1 0,0,0)'	(m _y 0,0,0)'

The translational subgroup of the subgroup D = 3.1.8 P2 of F(D) = 10.4.52 P2/m' is generated by the translations (1|1,0,0), (1|0,1,0), and (1|0,0,1) and the coset representatives of this group D are (1|0,0,0) and (2_y|0,0,0), the unprimed coset representatives on the right. In *The Magnetic Group Tables*, listed for the group type 3.1.8 P2 one finds the identical two coset representatives. Consequently, there is no change in the coordinate system, i.e. t=(0,0,0) and a'=a, b'=b, and c'=c. In the

coordinate system of the magnetic group 10.4.52 P2/m', the coset representatives of its subgroup D = 3.1.8 P2 are identical with the standard set of coset representatives of the group type 3.1.8 P2 found in *The Magnetic Group Tables*.

Example 2: For the 3-dimensional magnetic space group type 16.7.105 P_{2c} 22'2' one finds in *The Magnetic Group Tables*:

Serial		Non-primed Subgroup	
Number	Symbol	of Index Two	Standard Set of Coset Representatives

16.7.105 P_{2c} 22'2' P222₁ (0,0,0;a,b,2c) (1|0,0,0) (2_x|0,0,0) (2_y|0,0,1) (2_z|0,0,1)

The translational subgroup of the subgroup D = $17.1.106 P222_1$ of F(D) = $16.7.105 P_{2c} 22'2'$ is generated by the translations (1|1,0,0), (1|0,1,0), and (1|0,0,2) and the coset representatives of this group are all those coset representatives on the right. This subgroup D is of type 17.1.106 P222₁. In *The Magnetic Group Tables*, listed for the group type 17.1.106 P222₁ one finds a different set of coset representatives:

(1|0,0,0) $(2_x|0,0,0)$ $(2_y|0,0,\frac{1}{2})$ $(2_z|0,0,\frac{1}{2})$

Consequently, to show the relationship between this subgroup D of F(D) and the listed representative group of the group type 17.1.106 P222₁ in *The Magnetic Group Tables*, we change the coordinate system in which D is defined to (0,0,0;a,b,2c). In this new coordinate system the coset representatives of the subgroup D are identical with the coset representatives of the representative group of the group type 17.1.106 P222₁.

1: Survey of Magnetic Groups

Example 3: For the 3-dimensional magnetic space group type 18.4.116 $P2_12_1'2'$ one finds in *The Magnetic Group Tables*:

Serial Number	Non-primed Subgroup er Symbol of Index Two		Standard Set of Coset Representatives
18.4.116	P2 ₁ 2 ₁ '2'	P2 ₁ (0,¼,0 ;c,a,b)	$(1 000) (2_x \frac{1}{2},\frac{1}{2},0) (2_y \frac{1}{2},\frac{1}{2},0)' (2_z 000)'$

The translational subgroup of D is generated by the translations (1|1,0,0), (1|0,1,0), and (1|0,0,1) and the coset representatives of this group are (1|000) and $(2_x|1/2,1/2,0)$, the unprimed coset representatives on the right. The group D is of type 4.1.15 P2₁. In *The Magnetic Group Tables*, for the magnetic group type 4.1.15 P2₁ one finds a different set of coset representatives, (1|0,0,0) and $(2_y|0,1/2,0)$. Consequently, to show the relationship between the subgroup D of F(D) and the listed representative group of the group type 4.1.15 P2₁, we change the coordinate system in which the subgroup D is defined to (0,1/4,0;c,a,b). The origin is first translated from O to O+t , where t=(0,1/4,0)and the a new set of basis vectors, a'=c, b'=a, and c'=b are defined. In this new coordinate system the coset representatives of the subgroup D are identical with the standard set of coset representatives of the representative group of the group type 4.1.15 P2₁.

Section 2. Tables of Properties of Magnetic Groups Section 2: Tables of Properties of Magnetic Groups

In this section we present a guide to the tabulation of properties of the 1-, 2-, and 3-dimensional magnetic subperiodic groups and magnetic space groups given in the *Tables of Properties of Magnetic Groups* in *The Magnetic Group Tables*. The format and content of these magnetic group tables are similar to the format and content of the space group tables in *ITC-A*¹⁸, of the subperiodic group tables in the *ITC-E*¹³, and used in previous compilations of magnetic subperiodic groups⁴⁰ and magnetic space groups⁴¹. The content of the Tables of Properties of Magnetic Groups consists of: First page:

- (1) Lattice Diagram
- (2) Headline
- (3) Diagrams of symmetry-elements and of the general-positions
- (4) Origin
- (5) Asymmetric unit
- (6) Symmetry operations

Subsequent pages

- (7) Abbreviated headline
- (8) Generators selected
- (9) General and Special positions with spins (magnetic moments)
- (10) Symmetry of special projections

2.1 Lattice Diagram

For each three-dimensional magnetic space group, a three-dimensional lattice diagram is given In the upper left hand corner of the first page of the tables of properties of that group. (For all other magnetic groups, the corresponding lattice diagram is given within the symmetry diagram, see Section 2.3 below.) This lattice diagram depicts the coordinate system used, the conventional unit cell of the space group F, the magnetic space group's magnetic superfamily type, and the generators of the translational subgroup of the magnetic space group. For example, in Figures 2.1.1 and 2.1.2 we show the lattice diagrams for the orthorhombic magnetic space group



= $Pmc2_1$ ($Pca2_1$).

types 26.1.168 Pmc2₁ and 26.10.177 P_{2b} m'c'2₁, respectively. The generating lattice vectors depicted are color coded. Those colored black are not coupled with time inversion while those colored red are coupled with time inversion. In the former group 26.1.168 Pmc2₁, a magnetic group of the type F, the lattice is an orthorhombic "P" lattice, see Figure 2.1.1, and no generating translation is coupled with time inversion. In the latter group 26.10.177 P_{2b} m'c'2₁, a magnetic group of type M_R , the lattice is an orthorhombic "P_{2b}" lattice, see Figure 2.1.2, with the generating lattice vector in the y-direction coupled with time inversion.

2.2 Heading

Each table begins with a headline consisting of two lines with five entries. For 3dimensional magnetic space groups, this headline is to the right of the lattice diagram, an example is given in Figure 2.2.1:

P4/m'mm	4/m'mm	Tetragonal			
123.3.1001	P4/m'2'/m2'/m				
Figure 2.2.1: Headline of 3-dimensional magnetic space group 123.3.1001 P4/m'mm.					

On the upper line, starting on the left, are three entries:

(1) The *short international* (Hermann-Mauguin) *symbol* of the magnetic space group. Each symbol has two meanings: The first is that of the Hermann-Mauguin symbol of a magnetic space group type. The second is that of a specific magnetic

space group, the representative magnetic space group (see Section 1.2), which belongs to this magnetic space group type. Given a coordinate system, this group is defined by the list of symmetry operations (see Section 2.6) given on the page with this Hermann-Mauguin symbol in the heading, or by the given list of general positions and magnetic moments (see Section 2.9).

(2) The *short international* (Hermann-Mauguin) *point group symbol* for the geometric class to which the magnetic space group belongs.

(3) The crystal system or crystal system/Bravais system classification (See Table1.2) to which the magnetic space group belongs.

The second line has two additional entries:

(4) The three part numerical serial index of the magnetic group (see Section1.2.1).

(5) The *full international (Hermann-Mauguin) symbol* of the magnetic space group.

2.3 Diagrams of symmetry-elements and of general-positions

There are two types of diagrams, symmetry-elements diagrams and generalpositions diagrams. The symmetry-elements diagrams show (1) the relative locations and orientations of the symmetry elements and (2) the absolute locations and orientations of these symmetry elements in a given coordinate system. The generalpositions diagrams show, in that coordinate system, the arrangement of a set of symmetrically equivalent general points and the relative orientations of magnetic moments on this set of points .

All diagrams of 3-dimensional magnetic space groups and 3-dimensional subperiodic groups are orthogonal projections. The projection direction is along a basis vector of the conventional crystallographic coordinate system, see Table 1.1. If the other basis vectors are not parallel to the plane of the diagram, they are indicated by a subscript "p", e.g. a_p , b_p , and c_p . Schematic representations of the diagrams, showing their conventional coordinate systems, i.e. the origin "O" and basis vectors, are given in Table 2.1. For 2-dimensional magnetic space groups and magnetic frieze groups, the diagrams are in the plane defined by the groups conventional coordinate system.

The graphical symbols used in the symmetry-elements diagrams are listed in Table 2.2 and are an extension of those used in *ITC-A*¹⁸, *ITC-E*¹³ and Litvin⁴⁰. For



symmetry planes and symmetry axes parallel to the plane of diagram, for rotoinversions and for centers of symmetry, the "heights" h along the projection direction above the plane of the diagram are given. The heights are given as fractions of the shortest translation along the projection direction and if different from zero, are printed next to the graphical symbol, see e.g. Figure 2.3.1.

In the general-positions diagrams, the general positions and corresponding magnetic moments are color coded. Positions with a z-component of "+z" are circles color coded red and with a z-component of "-z" are circles color coded blue If the z-component is either "h+z" or "h-z" with h \neq 0, then the height "h" is printed next to the general position, e.g. $\frac{1}{4}$, see Figure 2.3.2. If two general positions have the

same x-component and y-component and z-components +z and -z, respectively, the



For magnetic groups M_R , of the type F(D) where D is an equi-class subgroup of F, the general-positions and symmetry-elements diagrams do not encompass, in all cases, the conventional unit cell of the non-primed subgroup D of the magnetic space group. For the symmetry-elements diagram, there is no necessity for explicitly enlarging the diagram as the symmetry-elements diagram is periodic with respect to all translations of the space group F of the magnetic space group F(D)^{49,50}. The general-positions diagram, in such cases, can be easily enlarged as one knows the translations of the magnetic space group, i.e. the general-positions diagram is periodic in the direction of the non-primed translations and in the direction of primed translations the magnetic moments are inverted. See diagrams of the group 51.15.401 P_{2b}m'ma' in Figure 2.3.3.

For magnetic space groups of the type F1', the symmetry-elements diagram is that of the group F. That each symmetry element also appears coupled with time inversion is represented by a red **1'** printed between and above the general-positions and symmetry-elements diagrams. Because groups of this type contain the time inversion





symmetry, the magnetic moments are all identically zero, and no arrows appear in the general- positions diagram. An example, the diagrams of magnetic space group $91.2.765 P4_{1}221'$, is shown in Figure 2.3.4.



For triclinic, monoclinic/oblique, monoclinic/rectangular, and orthorhombic rod groups the color coding of general-positions is extended according to the positive or negative values of the x and z components of the coordinates of the generalpositions. This color coding is:

red	for	x> 0	and	z> 0	
blue	for	x> 0	and	z< 0	
green for	x< 0	and	z> 0		
brown	for	x< 0		and	z< 0

Figure 2.3.5 shows an example of this color coding.

2.4 Origin

The choices of origin follow choices made in the *International Tables for Crystallography, Vol. A*¹⁸ *and Vol. C*¹³. If the magnetic space group is centrosymmetric then the inversion center or a position of high site symmetry, as on the four-fold axis of tetragonal groups, is chosen as the origin. For noncentrosymmetric groups, the origin is at a point of highest site symmetry. If no site symmetry is higher than 1, the origin is placed on a screw axis, a glide plane or at the intersection of several such symmetries.

In the *Origin* line below the diagrams, the site symmetry of the origin is given. An additional symbol indicates all symmetry elements that pass through the origin. For example, for the magnetic space group 140.1.1196 l4/mcm, one finds " **Origin** at center (4/m) at $4/mc2_1/c$." The site symmetry is 4/m and in addition, two glide planes

perpendicular to the y- and z-axis, and a screw axis parallel to the z-axis pass through the origin.

2.5 Asymmetric Unit

An asymmetric unit is a simply connected smallest part of space which, by application of all symmetry operations of the magnetic group, exactly fills the whole space. For subperiodic groups, because the translational symmetry is of a lower dimension than that of the space, the asymmetric unit is infinite in size. The asymmetric unit for subperiodic groups is defined by setting the limits on the coordinates of points contained in the asymmetric unit. For example, the asymmetric unit for the layer group 32.3.199 pm'2₁n' is:

Asymmetric unit $0 \le x \le \frac{1}{2}$; $0 \le y \le 1$; $0 \le z$

Since the translational symmetry of a magnetic space group is of the same dimension as that of the space, the asymmetric unit is a finite part of space. The asymmetric unit is defined, as above, by setting the limits on the coordinates of points contained in the asymmetric unit. For example, for the magnetic space group 140.3.1198 I4/m'cm one finds:

Asymmetric unit $0 \le x \le \frac{1}{2}; 0 \le y \le \frac{1}{2}; 0 \le z \le \frac{1}{4}; y \le \frac{1}{2} - x$

Drawings showing the boundary planes of the asymmetric unit occurring in the tetragonal, trigonal, and hexagonal systems, together with their algebraic equations are

given in Figure 2.8.1 of *ITC-A*¹⁸. Drawings of asymmetric units for cubic groups have been published by Koch & Fisher ⁴³. The asymmetric units have complicated shapes in the trigonal, hexagonal, and cubic crystal systems and consequently are also specified by giving the vertices of the asymmetric unit. For example, for the magnetic space group 176.1.1374 P6₃/m one finds:

Asymmetric unit	0 <u><</u> x <u><</u> 2/3;	0 <u><</u> y	<u><</u> 2/3;	0 <u><</u> z <u><</u> 1/4;	
	x <u><</u> (1+y)/2;	y <u><</u> m	in(1-x,(1+x)/2))	
Vertices	0,0,0	1/2,0,0	2/3,1/3,0	1/3,2/3,0	0,1/2,0
	0,0,1/4	1/2,0,1/4	2/3,1/3,1/4	1/3,2/3,1/4	0,1/2,1/4

Because the asymmetric unit is invariant under time inversion, all magnetic space groups F, F1', and F(D) of the magnetic superfamily of type F have identical asymmetric units, the asymmetric unit of the group F¹⁸.

2.6 Symmetry operations

Listed under the heading of *Symmetry operations* is the geometric description of the symmetry operations of the magnetic group. A symbol denoting the geometric description of each symmetry operation is given. Details of this symbolism, except for the use of prime to denote time inversion, are given in Section 11.2 of *ITC-A*¹⁸. For glide planes and screw axes the glide and screw part are always explicitly given in parentheses by fractional coordinates, i.e. by fractions of the basis vectors of the
coordinate system of F of the superfamily of the magnetic group. A coordinate triplet indicating the location and orientation of the symmetry element is given, and for rotoinversions, the location of the inversion point is also given. These symbols, with the addition of a prime to denote time inversion, follow those used in *ITC-A*¹⁸, *ITC-E*¹³, and Litvin^{40,41}. In addition, each symmetry operation is also given in Seitz notation ¹⁹, (see Section 1.2.3) see Figure 2.6.1 for an example, the symmetry operations of the magnetic space group 51.14.400 P_{2b}mma'.

Symmetry Operations				
For (0,0,0) + set				
(1) 1	(2) 2 1/4,0,z	(3) 2' 0,y,0	(4) 2' (1/2,0,0) x,0,0	
(1 0,0,0)	(2 _z 1/2,0,0)	(2 _y 0,0,0)'	(2 _x 1/2,0,0)'	
(5) 1'	(6) a' (1/2,0,0) x,y,0	(7) m x,0,z	(8) m 1/4,y,z	
(1 0,0,0)'	(m _z 1/2,0,0)'	(m _y 0,0,0)	(m _x 1/2,0,0)	
	For (0,	1,0)' +set		
(1) t' (0,1,0)	(2) 2' 1/4,1/2,z	(3) 2 (0,1,0) 0,y,0	(4) 2 (1/2,0,0) x,1/2,0	
(1 0,1,0)'	(2 _z 1/2,1,0)'	(2 _y 0,1,0)	(2 _x 1/2,1,0)	
(5) 1 0,1/2,0	(6) n (1/2,1,0) x,y,0	(7) m' x,1/2,z	(8) b (0,1,0) 1/4,y,z	
(1 0,1,0)	(m _z 1/2,1,0)	(m _y 0,1,0)'	(m _x 1/2,1,0)'	
Figure 2.6.1: Symmetry operations of magnetic space group 51.14.400 P _{2b} mma'.				

The corresponding coordinate triplets of the *General positions*, see Section 2.9, may be interpreted as a second description of the symmetry operations, a description in matrix form. The numbering (1), (2), ..., (p), ... of the entries in the blocks *Symmetry operations* is the same as the numbering of the corresponding coordinate triplets of the *General positions*, the first block below *Positions*. For all magnetic groups with primitive "P" lattices, the two lists, *Symmetry operations* and *General positions*, have the same number of entries.

For magnetic groups with centered cells, only one block of several (2,3, or 4) blocks of the *General positions* is explicitly given, see Figure 2.6.2. A set of (2,3, or 4) centering translations is given below the subheading *Coordinates*. Each of these translations is added to the given block of *General positions* to obtain the complete set of blocks of *General positions*. While only one of the several blocks of *General positions* is explicitly given, the corresponding symmetry operations of all blocks are explicitly given under *Symmetry operations*. Each corresponding block of symmetry operations is listed under a subheading of "centering translation + set" for each centering translation listed below the subheading *Coordinates* under *General positions*.

Positions		Coordinates		
	(0,0,0)	+ (0,1,0)'		
16 I 1 (1) x,y,z [u,v,w]	(2) \overline{x} +1/2, \overline{y} ,z [\overline{u} , \overline{v} ,w]	(3) $\overline{x}, y, \overline{z} [u, \overline{v}, w]$	(4) x+1/2, y, z [u,v,w]	
(5) $\overline{x}, \overline{y}, \overline{z} [\overline{u}, \overline{v}, \overline{w}]$	(6) x+1/2,y, z [u,v,w]	(7) x, \overline{y} , z [\overline{u} , v, \overline{w}]	(8) x+1/2,y,z [u, v,w]	
Figure 2.6.2: General positions of magnetic space group 51,14,400 Pamma'.				

One will find among the equi-class three-dimensional magnetic space groups M_R = F(D) sets of groups which have identical entries under *Symmetry operations*. The translational elements of a group $M_R = F(D)$ consists of the translations $T_R^M = T^D + t_a^{-1} T^D$ where T^D is the translational subgroup of D, $T = T^D + t_a^{-}T^D$ the translational subgroup of F, and t_a is the chosen translation, see Tables 1.1, to characterize the translational subgroup T_R^M of M_R . In each set, the translation t_a is the same, while the translational groups T_R^M and T^D are unique. In Figure 2.6.3 we give an example of a set of three such groups, 25.6.160 P_{2a} mm2, 25.7.161 P_C mm2, and 25.9.163 P_F mm2 . For all three, the first block of symmetry operations is that of the common point group mm2. The second block consists of the symmetry operations of the first block, as t_a is the same translation chosen in $T_R^M = T^D + t_a^{-1} T^D$, see Tables 1.1. In Table 2.3 we list all sets of magnetic groups M_R where the choice of t_a in Tables 1.1 has led to identical Symmetry operations in the Tables of Properties of Magnetic Groups.

	Fc	or (0,0,0) + set	
(1) 1	(2) 2 0,0,z	(3) m x,0,z	(4) m 0,y,z
(1 0,0,0)	(2 _z 0,0,0)	(m _y 0,0,0)	(m _x 0,0,0)
	Fc	or (1,0,0)' + set	
(1) t' (1,0,0)	(2) 2' ½,0,z	(3) a' (1,0,0) x,0,z	(4) m' ½,y,z
(1 1,0,0)'	(2 _z 1,0,0)'	(m _y 1,0,0)'	(m _x 1,0,0)'

Figure 2.6.3: Symmetry operations of the magnetic space groups 25.6.160 $\rm P_{2a}mm2,$ 25.7.161 $\rm P_{c}mm2,$ and 25.9.163 $\rm P_{F}mm2$.

2.7 Abbreviated headline

On the second and subsequent pages of the tables for a single magnetic group there is an abbreviated headline. This abbreviated headline contains three items: 1) the word "continued", 2) the three part number of the magnetic group type, and 3) the short international (Hermann-Mauguin) symbol for the magnetic group type.

2.8 Generators selected

The line *Generators selected* lists the symmetry operations selected to generate the symmetrically equivalent points of the *General positions* from a point with coordinates x, y, z. The first generator is always the identity operation given by (1) followed by generating translations. Additional generators are given as numbers (p) which refer to the coordinate triplets of the *General positions* and to corresponding symmetry operations in the first block, if more than one, of *Symmetry operations*.

2.9 General and special positions with spins (magnetic moments)

The entries under *Positions*, referred to as *Wyckoff positions*, consists of the *General positions*, the upper block, followed by blocks of *Special positions*. The upper block of positions, the *General positions*, is a set of symmetrically equivalent points where each point is left invariant only by the identity operation or, for magnetic groups F1', by the identity operation and time inversion, but by no other symmetry operations of the magnetic group. The lower blocks, the special positions, are sets of symmetrically

equivalent points where each point is left invariant by at least one additional operation in addition to the identity operation, or, for magnetic space groups F1', in addition to the identity operation and time inversion.

For each block of positions the following information is provided:

Multiplicity: The multiplicity is the number of equivalent positions in the conventional unit cell of the non-primed group F associated with the magnetic group.

Wyckoff Letter: This letter is a coding scheme for the blocks of positions, starting with "a" at the bottom block and continuing upwards in alphabetical order.

Site symmetry: The site symmetry group is the largest subgroup of the magnetic space group that leaves invariant the first position in each block of positions. This group is isomorphic to a subgroup of the point group of the magnetic group. An "oriented" symbol is used to show how the symmetry elements at a site are related to the conventional crystallographic basis and the sequence of characters in the symbol correspond to the sequence of symmetry directions in the magnetic group symbol, see Table 1.3 . Sets of equivalent symmetry directions that do not contribute any element to the site symmetry are represented by dots. Sets of symmetry directions having more than one equivalent direction may require more than one character if the site-symmetry group belongs to a lower crystal system. For example, for the 2c position of the magnetic space group P4'm'm (99.3.825) the site symmetry group is " 2m'm'. " where the two characters m'm' represent the secondary set of tetragonal symmetry directions.

Coordinates of Positions and Components of Magnetic Moments : In each block of positions, the coordinates of each position are given. Immediately following each set of position coordinates are the components of the symmetry allowed magnetic moment at that position. The components of the magnetic moment of the first position is determined from the given site symmetry group. The components of the magnetic moments at the remaining positions are determined by applying the symmetry operations to the components of that magnetic moment at the first position.

2.10 Symmetry of special projections

The symmetry of special projections is given for the representative groups of all two and three dimensional magnetic space group types and magnetic subperiodic group types. For each three dimensional group, the symmetry is given for three projections, projections onto planes normal to the projection directions. If there are three symmetry directions, see Table 1.3, the three projection directions correspond to primary, secondary, and tertiary symmetry directions. If there are less than three symmetry directions, the additional projection direction or directions are taken along coordinate axes. For two dimensional groups, there are two orthogonal projections. The projections are onto lines normal to the projection directions.

The projection directions and the resulting types of symmetry groups of the projections are as follows:

3-dimensional Magnetic Space Groups			
Triclinic	[001]	Two-dimensional Magnetic Space Group	
Monoclinic	[100]	Two-dimensional Magnetic Space Group	
Orthorhombic	[010]	Two-dimensional Magnetic Space Group	
Tetragonal	[001]	Two-dimensional Magnetic Space Group	
	[100]	Two-dimensional Magnetic Space Group	
	[110]	Two-dimensional Magnetic Space Group	
Hexagonal	[001]	Two-dimensional Magnetic Space Group	
Rhombohedral	[100]	Two-dimensional Magnetic Space Group	
	[210]	Two-dimensional Magnetic Space Group	
Cubic	[001]	Two-dimensional Magnetic Space Group	
	[111]	Two-dimensional Magnetic Space Group	
	[110]	Two-dimensional Magnetic Space Group	

2-dimensional Magnetic Space Groups

Oblique[10]	One-dimensional Magnetic Space Group	
Rectangular [01]	One-dimensional Magnetic Space Group	

Square[10]	One-dimensional Magnetic Space Group
[11]	One-dimensional Magnetic Space Group
Hexagonal[10]	One-dimensional Magnetic Space Group
[21]	One-dimensional Magnetic Space Group
Layer Groups	
Triclinic/Oblique Monoclinic/Oblique Monoclinic/Rectangular	
Orthorhombic/Rectangular [001]	Two-dimensional Magnetic Space Group
[100]	Magnetic Frieze Group
[010]	Magnetic Frieze Group
Tetragonal/Square[001]	Two-dimensional Magnetic Space Group
[100]	Magnetic Frieze Group
[110]	Magnetic Frieze Group
Trigonal/Hexagonal	
Hexagonal/Hexagonal[001]	Two-dimensional Magnetic Space Group
[100]	Magnetic Frieze Group
[210]	Magnetic Frieze Group

Rod Groups

Triclinic Monoclinic/Oblique Monoclinic/Rectangular Orthorhombic[001] Two-dimensional Magnetic Point Group

[100] Magnetic Frieze Group

[010] Magnetic Frieze Group

Tetragonal[001] 1	Two-dimensional Magnetic Point Group
[100] [Magnetic Frieze Group
[110] [Magnetic Frieze Group
Trigonal Hexagonal[001] ٦	Two-dimensional Magnetic Point Group
[100] [Magnetic Frieze Group
[210] [Magnetic Frieze Group

Frieze Groups

Oblique[10]	One-dimensional Magnetic Point Group
-------------	--------------------------------------

The international (Hermann-Mauguin) of the symmetry group of each projection is given. Below this symbol, the basis vector(s) of the projected symmetry group and the origin of the projected symmetry group are given in terms of the basis vector(s) of the projected magnetic group. The location of the origin of the symmetry group of the projection is given with respect to the unit cell of the magnetic group from which it has been projected.

Section 3: OG/BNS Magnetic Group Type Symbols

Section 3: OG/BNS Magnetic Group Type Symbols

We consider in this section the difference between the magnetic group type symbols of the three-dimensional magnetic space groups introduced by Opechowski and Guccione ^{36,37} (OG symbols) and the symbols for three-dimensional two color space group types used by Belov, Nerenova, and Smirnova⁴² (BNS symbols) which are also used for symbols of three-dimensional magnetic space group types ³⁴.

Groups in the reduced magnetic superfamily of a group F, see Section 1.1, were divided into 1) the group F, 2) the group F1', and 3) non-equivalent groups of the form F(D). The third was subdivided into groups M_T and M_R , groups where D is an equitranslational subgroup and equi-class subgroup, respectively, of F. The OG and BNS symbols for group types F , F1', and M_T are the same. For groups M_R the OG group type symbol for F(D) is based on the group type symbol for the group F (see Opechowski and Litvin⁴²) while the BNS group type symbol for F(D) is based on the group type symbol for the group D: A group M_R can be written as $M_R = D + t_{\alpha}' D$ where t_{α} is a translation of F not contained in D. A BNS group type symbol for groups M_{R} is the group type symbol of D with the translation t_a either denoted or implied by a subindex on the letter representing the translational subgroup of D. For example, the threedimensional magnetic space group is F(D) = 30.7.211 Pnc2(Pnn2). The OG group type symbol is 30.7.211 P_{2a} nc'2' is based on the symbol of the group F = 30.1.205 Pnc2, where the subindex on the translational group symbol and the primes denote operations which are coupled with time inversion ⁴². The BNS symbol is P_ann2, based on the

Section 3: OG/BNS Magnetic Group Type Symbols

symbol of the group D = 34.1.231 Pnn2, and where the translation t_{α} is denoted by the subindex "a" on the letter P representing the translational subgroup of D.

In the Comparison of OG and BNS Magnetic Group Type Symbols , in The Magnetic Group Tables, only M_R group type symbols are listed separately in both OG and BNS notation since for group types F, F1', and M_T the group type symbols are the same. In Figure 3.1 we list examples from *The Magnetic Group Tables* of M_R magnetic group type symbols with the addition of the F(D) notation for the magnetic group type symbol.

 Figure 3.1: Examples of comparisons of OG and BNS symbols for three-dimensional

 F(D) magnetic space groups. The OG symbol is based on the symbol of the group F and the BNS symbol on the symbol of the group D.
 OG
 BNS
 F(D)

 30.7.211
 P_{2a}nc'2'
 P_ann2
 Pnc2(Pnn2)

 38.12.276
 A_Pm'm'2
 P_Anc2
 Amm2(Pnc2)

Secction 4. Maximal Subgroups of Index < 4

Section 4: Maximal Subgroups of Index < 4

We consider the maximal subgroups of index \leq 4 of the representative groups of the 1-,2-, and 3-dimensional magnetic space group types and the 2- and 3-dimensional magnetic subperiodic group types. A complete listing of the maximal subgroups of the representative groups of the 2- and 3-dimensional space group types can be found in *ITC-A1*⁴⁴. The maximal subgroups of index \leq 4 of the representative groups of the 3-dimensional space groups and layer and rod groups can also be found on the Bilbao Crystallographic Server⁴⁵.

For magnetic groups, an abstract of a method to determine the maximal subgroups of magnetic groups was published by Sayari & Billiet⁴⁶. The maximal subgroups of magnetic groups found in *The Magnetic Group Tables*, were derived⁴⁷ using a method given by Litvin⁴⁸. As an example, We consider the maximal subgroups of index \leq 4 of the magnetic space group 55.5.445 Pb'a'm. In *The Magnetic Group Tables*, for the maximal subgroups of this magnetic space group one first finds, in bold blue type, information which defines the representative group of this type:

55.5.445 Pb'a'm (0, 0, 0; a,b,c) (1|000) $(2_x|^{\frac{1}{2}})'$ $(2_y|^{\frac{1}{2}})'$ $(2_z|000)$ ($\overline{1}|000$) $(m_x|^{\frac{1}{2}})'$ $(m_y|^{\frac{1}{2}})'$ $(m_z|000)$

The first column gives the serial number of the group, followed in the second column by its symbol. The third column gives the origin and basis vectors of the conventional unit cell of the non-primed translational subgroup of this magnetic group. The coset

Secction 4. Maximal Subgroups of Index \leq 4

representatives of this representative group are given on the right. Following this is the list of the maximal subgroups of index \leq 4 of this magnetic space group. For example, one finds listed the equi-translational subgroup of the type 32.4.222 Pb'a'2:

Pb'a'2 2 (0, 0, 0; a, b, c) (1|000) (2_z|000) ($m_y|_{21/2}^{1/2}0$)' ($m_x|_{21/2}^{1/2}0$)'

The second column gives the index of the subgroup. In the third column is the change in coordinates, if required, to have the coset representatives of the the listed subgroup become identical with the coset representatives of the representative group of that subgroup type. In this case, the coset representatives on the right are identical with the coset representative group 32.4.222 Pb'a'2. Consequently, the coset representatives of the subgroup 32.4.222 Pb'a'2 in the coordinate system of 55.5.445 Pb'a'm are the same as those of the representative group 32.4.222 Pb'a'2. Therefore one finds (0, 0, 0;a,b,c) in the third column signifying that no coordinate transformation is necessary.

That the coset representatives of the subgroup are the same as those of the representative group of that type is not always the case. For example, A second subgroup is the equi-class subgroup of the type 32.4.222 Pb'a'm:

The coset representatives of this subgroup are not the same as the coset representatives

Secction 4. Maximal Subgroups of Index \leq 4

of the representative group 32.4.222 Pb'a'm where the z-component of the non-primitive translation associated with all coset representatives is zero. To have the coset representatives of this subgroup be identical with the coset representatives of the standard representative group of 32.4.222 Pb'a'm one must change the origin of the coordinate system. This information is provided in the symbol (0, 0, $\frac{1}{2}$;a,b,2c) where $0,0,\frac{1}{2}$ denotes the new origin. Note also that the "a,b,2c" defines the conventional unit cell of the translational group of this non-primed group.

To have the coset representatives of the subgroup be identical with the coset representatives of the representative group of the same type may require a change in the coordinate system setting. For example the subgroup 10.1.49 P2/m of 32.4.222 Pb'a'm:

P2/m 2 (0, 0, 0;b,c,a) (1|000) ($2_z|000$) ($\overline{1}|000$) ($m_z|000$)

The coset representatives of the representative group 10.1.49 P2/m are:

(1|000) (2_v|000) ($\overline{1}$ |000) (m_v|000)

The change in setting to have the coset representatives of the subgroup be identical with the coset representatives of the representative group 10.1.49 P2/m is given in (0, 0, 0;b,c,a), i.e. changing the setting from a,b,c to b,c,a. Other cases may require a simultaneous change in both the origin and the coordinate system setting.

In the tabulations of the maximal subgroups of the representative groups of the type F1' not all maximal subgroups are explicitly listed. The maximal subgroup F of F1' is

Secction 4. Maximal Subgroups of Index \leq 4

not listed. If G is a maximal subgroup of F, then G1' is a maximal subgroup of F1' but is also not explicitly listed. All maximal subgroups G of F are listed under F, and consequently, all maximal subgroups G1' of F1' are then found from that list of all maximal subgroups G of F, by multiplying each by 1'. Also, in the listing of the coset representatives of a group F1' itself, only the coset representatives of the group F are explicitly listed. The second not listed set is found by "priming" each coset representative of the first set , i.e. multiplying each with 1'.

- 1. Speiser, A., *Die Theorie der Gruppen von endlicher Ordnung*, 4th ed.(Birkhauser, Basel). 1st ed. (Springer, Berlin, 1924), 2nd ed. (Springer, Berlin, 1927).
- 2. Hermann, C., Z. Kristallogr. **69** 259-270 (1929).
- 3. Alexander, E., Z. Kristallogr. **70** 367-382 (1929).
- 4. Alexander, E., Z. Kristallogr. **89** 606-607 (1934).
- 5. Herrmann, K., Z. Kristallogr. **69** 226-229 (1929).
- 6. Alexander, E, & Herrmann, K., Z. Kristallogr. **70** 328-345 (1929).
- 7. Alexander, E, & Herrmann, K., Z. Kristallogr. **69** 285-299 (1929).
- 8. Weber, L., Z. Kristallogr. **70** 309-327 (1929).
- 9. Heesch, H., Z. Kristallogr. **71** 95-102 (1929).
- 10. Heesch, H., Z. Kristallogr. 72 177-201 (1929).
- 11. Holser, W.T., Z. Kristallogr. **110** 266-281 (1958).
- 12. Wood, E.A., Bell Syst. Tech. J. **43** 541-559 (1964).
- 13. *International Tables for Crystallography,* Vol. E: Subperiodic Groups, edited by V. Kopsky and D. B. Litvin. New York: Wiley (Second Edition 2010).
- 14. Shubnikov, A.V. & Koptsik, V.A. (1974). *Symmetry in Science and Art*, New York: Plenum Press.
- 15. Fedorov, E.S. *Symmetry of regular systems of figures*, Proc. St. Petersburg Mineral. Soc. 28. pp. 1-146 (1891) [in Russian.]
- 16. Schoenfliess, A.M. Kristallsysteme und Kristallstructur (Teubner, Leipzig) (1891)
- 17. Barlow, W., Z. Krist. Min. 23, pp. 1-63 (1894).
- 18. *International Tables for Crystallography,* Vol. A: Space Groups, edited by Th. Hahn. Dordrecht: Klewer Academic Publishers. (Fifth edition 2002).

- 19. Burns, G. & Glazer, A.M., Space Groups for Solid State Scientists, 2nd Edition (Academic Press, New York, (1990)).
- 20. Landau, L.I. & Lifschitz, E.M. (1951). *Statistical Physics*, Gostekhizdat, Moscow (in Russian); English Translation, Pergamon Press, Oxford (1958).
- 21. Landau, L.I. & Lifschitz, E.M. (1957). *Electrodynamics of Continuous Media*, Gostekhizdat, Moscow (in Russian); English Translation, Addison-Wesley, Reading, MA. (1960).
- 22. Heesch, H. (1930). Z. fur Kristallogr. **73**, 325-345.
- 23. Shubnikov, A.V., Belov, N.V. & others, *Colored Symmetry*, (Oxford: Pergamon Press (1964)).
- Belov, N.V., Kristallografiya 1 474-476 (1956).(in Russian), English translation in Soviet Physics - Crystallography 1 372-374 (1956); see also reference (23) pp. 222-227.
- 25. Neronova, N.N. & Belov, N.V., Kristallografiya **6** 3-12 (1961). (in Russian), English translation in Soviet Physics - Crystallography **6** 1-9 (1961).
- Galyarskii, E.I. & Zamorzaev, A.M., Kristallografiya **10** 147-154 (1965). (in Russian). English translation in Soviet Physics - Crystallography 10 109-115 (1965).
- 27. Shubnikov, A.V., Kristallografiya **4** 279-285 (1959), (in Russian). English translation in Soviet Physics Crystallography 4 261-266 (1959).
- Palistrant, A.F. & Zamorzaev, A.M., Kristallografiya 9 155-161 (1964), (in Russian). English translation in Soviet Physics - Crystallography 8 123-128 (1964).
- 29. Cochran, W. Acta Crystallographica **5**, 630-633 (1952).
- 30. Zamorzaev, A.M. (1953). *Dissertation* (in Russian), Leningad State University.
- 31. Zamorzaev, A.M. (1957). *Kristallografiya* **2** 15-20: English Translation *Soviet Phys. Cryst.* **2** 10-15.
- Belov, N.V., Neronova, N.N, & Smirnova, T.S. (195 7). Sov. Phys. Crystallogr. 1, 487-488. see also (1955). Trudy Inst. Krist. Acad. SSSR 11 33-67 (in Russian). English translation in by A.V. Shubnikov, N.V. Belov and others (1964).

- 33. Zamorzaev, A.M. (1976). *The Theory of Simple and Multiple Antisymmetry*, Kishinev: Shtiintsa. (in Russian).
- Koptsik, V.A, Shubnikov Groups. Handbook on the Symmetry and Physical Properties of Crystal Structures (Izd. M.G.U., Moscow (1966) (in Russian). (English translation of text: J. Kopecky & B.O. Loopstra, Fysica Memo 175, Stichting, Reactor Centrum Nederland, (1971)).
- 35. Zamorzaev, A.M. & Palistrant, A.P. (1980). Zeit. fur Krist. **151** 231-248.
- 36. Opechowski, W. & Guccione, R., *Magnetism*, edited by G.T. Rado & H. Suhl, Vol. 2A, ch.3, (New York: Academic Press. (1965)).
- 37. Opechowski, W., *Crystallographic and Metacrystallographic Groups*, (Amsterdam: North Holland (1986)).
- 38. Litvin, D.B., Acta Crystallographica, **A55**, 963-964 (1999).
- 39. Litvin, D.B., Acta Crystallographica, **A57**, 729-730 (2001).
- 40. Litvin, D.B., Acta Crystallographica, **A61**, 382-385 (2005).
- 41. Litvin, D.B., Acta Crystallographica, **A64**, 419-424 (2008).
- 42. Opechowski, W. & Litvin, D.B., Ann. Phys. 2, 121-125 (1977).
- 43. Koch, E. & Fisher, W., Acta Cryst. **A30**, 490-496 (1974).
- 44. International Tables for Crystallography, Vol. A1: Relations between Space Groups, edited by H. Wondratschek & U. Muller. Dordrecht: Klewer Academic Publishers. (2004).
- Aroyo, M.I., Perez-Mato, J.M., Capillas, C., Kroumova, E., Ivantchev, S., Madariaga, G., Kirov, S. & Wondratschek, H., Z. Kristallogr. **221** 14-27 (2006). (see also <u>http://www.cryst.ehu.es</u>)
- 46. Sayari, A. & Billiet. Y., Acta Crystallographica. A33 985-986 (1977).
- 47. Litvin, D.B., Acta Crystallographica, A64 345-347 (2008).
- 48. Litvin, D.B., Acta Crystallographica, **A52** 681-685 (1996).
- 49. Kopsky, V., J. Math. Phys. **34** 1548-1556 (1993).

- 50. Kopsky. V., J. Math. Phys. **34** 1557-1576 (1993).
- 51. Litvin, D.B. & Kopsky, V. Acta Crystallographica A67 415-418 (2011).

Tables

Table 1.1: Translational subgroups of magnetic groups

Translational subgroups denoted by a symbol consisting of a single letter with no subscripts are symbols of translational subgroups of magnetic groups **F**, **F1'** and **M**_T. A second symbol gives the generators of the translational group in the subscript of the corresponding translational group symbol. These generating translations are also shown as black arrows in the corresponding figure.

Translational subgroups denoted by a symbol consisting of a letter with a second letter or numeral and letter as subscripts are translational subgroups of magnetic groups \mathbf{M}_{R} . The translational subgroup of these groups are of the form $\mathbf{T}_{R}^{\mathsf{M}} = \mathbf{T}^{\mathsf{D}} + \mathbf{t}_{\alpha}' \mathbf{T}^{\mathsf{D}}$, where \mathbf{T}^{D} is the subgroup of index 2 of unprimed (not coupled with time inversion) translations of $\mathbf{T}_{R}^{\mathsf{M}}$. \mathbf{t}_{α}' is a primed translation of $\mathbf{T}_{R}^{\mathsf{M}}$, i.e. a translation of $\mathbf{T}_{R}^{\mathsf{M}}$ not in \mathbf{T}^{D} . Additional symbols are given which give the generating translations of \mathbf{T}^{D} as subscripts. The translation chosen for \mathbf{t}_{α} is also explicitly given. In the corresponding figures, generating translations which are in \mathbf{T}^{D} are shown in black and generating translations which are in $\mathbf{t}_{\alpha}' \mathbf{T}^{\mathsf{D}}$ are shown in red.



Table 1.1.1 Translational subgroups of 3-dimensional magnetic space groups



Monoclinic System (2-fold axis along y)







Orthorhombic System







 $\mathsf{A} = \mathsf{A}_{\mathsf{a},\mathsf{b},\frac{1}{2}(\mathsf{b}+\mathsf{c})}$

 $\mathsf{A}_{2\mathsf{a}} = \mathsf{A}_{2\mathsf{a},\mathsf{b},\mathsf{b+c}}$ $\mathbf{t}_{\alpha} = \mathbf{a} = (1,0,0)$

 $\mathbf{t}_{\alpha} = \frac{1}{2}(b+c) = (0,\frac{1}{2},\frac{1}{2})$

 $A_{I} = A_{2a,b,\frac{1}{2}(2a+b+c)}$ $\mathbf{t}_{\alpha} = \mathbf{a} = (1,0,0)$





 $F = F_{\frac{1}{2}(a+b),\frac{1}{2}(b+c),\frac{1}{2}(a+c)}$

 $\mathbf{t}_{\alpha} = \frac{1}{2}(a+c) = (\frac{1}{2}, 0, \frac{1}{2})$ $\mathbf{t}_{\alpha} = \frac{1}{2}(a+b) = (\frac{1}{2}, \frac{1}{2}, 0)$







 $\mathbf{t}_{\alpha} = \mathbf{a} = (1,0,0)$





y

Trigonal System (Rhombohedral Axes)



Tables

Trigonal System (Hexagonal Axes) Hexagonal System





Cubic System







Table 1.1.2 Translational subgroups of 2-dimensional magnetic layer groups and 2-dimensional magnetic space groups

Oblique System







y

Rectangular System



Tables



Square System





Hexagonal System



 Table 1.1.3 Translational subgroups of 3-dimensional magnetic rod groups, 2-dimensional

 magnetic frieze groups, and 1-dimensional magnetic space groups



Table 1.2 Relative lengths and mutual orientations of translation vectors of translational subgroups of magnetic groups

a, b, c respectively denote the lengths of generating translation vectors **a**, **b**, **c** of translational subgroups of magnetic groups. α , β , γ denote the angle between **b** and **c**, **a** and **c**, and **a** and **b**, respectively.

Table 1.2.1 3-dimensional magnetic space groups

Crystal system	Restrictions on conventional coordinate system	Cell Parameters to be determined
Triclinic	None	a, b, c, α, β, γ
Monoclinic	$\alpha = \gamma = 90^{\circ}$	a, b, c, γ
Orthorhombic	$\alpha = \beta = \gamma = 90^{\circ}$	a, b, c
Tetragonal	a = b; $\alpha = \beta = \gamma = 90^{\circ}$	a, c
Trigonal	Hexagonal axes: $a = b$ $\alpha = \beta = 90^{\circ}$, $\gamma = 120^{\circ}$	a, c
	Rhombohedral axes: $a = b = c$, $\alpha = \beta = \gamma$	a, α
Hexagonal	a = b $\alpha = \beta = 90^{\circ}$, $\gamma = 120^{\circ}$	а, с
Cubic	$a = b = c$, $\alpha = \beta = \gamma = 90^{\circ}$	а

Conventional Coordinate System

Table 1.2.2 2-dimensional magnetic space groups

Conventional Coordinate System	
--------------------------------	--

 Crystal system	Restrictions on conventional coordinate system	Cell Parameters to be determined
Oblique	None	a, b, γ
Rectagular	$\gamma = 90^{\circ}$	a, b
Square	$a = b$, $\gamma = 90^{\circ}$	а
Hexagonal	a = b , γ = 120°	а

Table 1.2.3 1-dimensional magnetic space groups

Conventional Coordinate System

Crystal system	Restrictions on conventional coordinate system	Cell Parameters to be determined
	None	а

Table 1.2.4 Magnetic layer groups

Conventional Coordinate System

 Crystal system	Restrictions on conventional coordinate system	Cell parameters to be determined
Triclinic	None	a, b, γ
Monoclinic/oblique	$\alpha = \gamma = 90^{\circ}$	a, b, γ
Monoclinic/rectangular	$\beta = \gamma = 90^{\circ}$	a, b
Orthorhombic	$\alpha = \beta = \gamma = 90^{\circ}$	a, b
Tetragonal	a = b; $\alpha = \beta = \gamma = 90^{\circ}$	а
Trigonal	a = b , α = β = 90° , γ = 120°	а
Hexagonal	a = b , α = β = 90° , γ = 120°	а

Table 1.2.5 Magnetic rod groups

Conventional Coordinate System

Crystal system	Restrictions on conventional coordinate system	Cell Parameters to be determined
Triclinic	None	С
Monoclinic/oblique	$\beta = \gamma = 90^{\circ}$	с
Monoclinic/rectangular	$\alpha = \beta = 90^{\circ}$	с
Orthorhombic	$\alpha = \beta = \gamma = 90^{\circ}$	с
Tetragonal	$\alpha = \beta = \gamma = 90^{\circ}$	с
Trigonal	$a=b$, $\alpha=\beta=90^{\circ}$, $\gamma=120^{\circ}$	с
Hexagonal	a = b , α = β = 90° , γ = 120°	с

Table 1.2.6 Magnetic frieze groups

	Conventional Coordinate System		
Crystal system	Restrictions on conventional coordinate system	Cell Parameters to be determined	
Oblique	None	а	
Rectangular	γ = 90°	а	

Table 1.3 Symmetry directions (positions in Hermann-Mauguin symbols)

Directions that belong to the same set of equivalent symmetry directions are collected between braces. The first entry in each set is taken as the representative of that set.

Table 1.3.1 3-dimensional magnetic space groups

Lattice	Primary	Secondary	Tertiary	
Triclinic	None			
Monoclinic	[010] unique axis b			
Orthorhombic	[100]	[010]	[001]	
Tetragonal	[001]	{[100]} {[010]}	{[110] {[110]}	
Hexagonal	[001]	{[100] {[010] [110]	{[110] [120] [210]	
Rhombohedral (hexagonal axes)	[001]	{[100] [010] [110]		
Cubic	{[100] [010] [001]	([11]) [[1]] [[1]] [[1]] [[1]] [[1]]	$\begin{cases} [1\overline{1}0] & [110] \\ [01\overline{1}] & [011] \\ [\overline{1}01] & [101] \\ \end{cases}$	
Table 1.3.2	2-dimensional	magnetic	space grou	ps
-------------	---------------	----------	------------	----
-------------	---------------	----------	------------	----

Lattice	Primary	Secondary	Tertiary
Oblique	Rotation point in plane		
Rectangular	Rotation point in plane	[10]	[01]
Square	Rotation point in plane	{[10] {[01]}	$ \begin{bmatrix} [1 \overline{1}] \\ [1 1] \end{bmatrix} $
Hexagonal	Rotation point in plane	$ \begin{cases} [10] \\ [01] \\ [\overline{1}\overline{1}] \end{cases} $	$ \left\{ \begin{matrix} [1\overline{1}] \\ [12] \\ [\overline{2}\overline{1}] \end{matrix} \right\} $

Table 1.3.3 1-dimensional magnetic space groups

Lattice	Primary
Linear	reflection through a point (inversion through a point)

Table 1.3.4 Magnetic layer groups and rod groups

Lattice	Primary	Secondary	Tertiary
Triclinic	None		
Monoclinic Orthorhombic	[100]	[010]	[001]
Tetragonal	[001]	{[100]} {[010]}	{[110] [110]∫
Trigonal Hexagonal	[001]	$ \begin{cases} [100] \\ [010] \\ [\overline{1}\overline{1}0] \end{cases} $	$ \begin{cases} [1\overline{1}0] \\ [120] \\ [\overline{2}\overline{1}0] \\ \end{cases} $

Table 1.3.5 Magnetic frieze groups

Lattice	Primary	Secondary	Tertiary
Oblique	Rotation point in plane		
Rectangular	Rotation point in plane	[10]	[01]

Table 1.4: Subindex symmetry directions and symbols

Table 1.4.1 3-Dimensional

Lattice	Symmetry direction	Subindex symbol	
Monoclinic	[010]	У	
Orthorhombic	[100]	x	
	[010]	У	
	[001]	Z	
Tetragonal	[001]	z	
0	[100]	X	
	[010]	y	
	[110]	x y	
	[110]	xý	



Hexagonal	[001] [100] [010] [110] [210] [120] [110]	z x y xy 1 2 3
Rhombohedral (hexagonal axes)	[001] [100] [010] [110]	z x y xy



Cubic	[100]	Х
	[010]	У
	[001]	Z
	[111]	XYZ
	[111]	xyz
	[11]	xyz
	[11]	xyz
	[110]	xy
	[110]	x y
	[011]	yz
	[011]	<u> </u>
	[101]	XZ
	[101]	xz



Table 1.4.2 2-Dimensional



Table 1.4.3 1-Dimensional

Lattice	Symmetry direction	Subindex symbol
Linear	[1]	x







Rhombohedral



 Table 2.1.2
 2-dimensional magnetic space groups

 Table 2.1.3
 1-dimensional Magnetic space groups















b_p

Ω

Monoclinic/rectangular



Orthorhombic



Tetragonal



Trigonal, Hexagonal











Table 2.2: Graphic Symbols

2.2.1 1-dimensional magnetic group symbols

Groups: 1-dimensional magnetic space groups



2.2.2 -dimensional magnetic group symbols

Groups: Frieze groups

2-dimensional magnetic space groups

Table 2.2.2.1: Symmetry lines in the plane

Symmetry line	Graphical symbol	Glide vectors in units of lattice translation vectors parallel to the plane	Printed symbol
mirror line		none	m
primed mirror line		none	m'
glide line		1/2 along line in plane	g
primed glide line		1/2 along line in plane	g'

Table 2.2.2.2: Symmetry points in the plane

Symmetry point	Graphical Symbol	Printed Symbol
two-fold rotation point	•	2
two-fold primed rotation point	•	2'
three-fold rotation axis		3
three-fold primed rotation axis		3'
four-fold rotation axis	•	4
four-fold primed rotation axis	•	4'
six-fold rotation axis	۲	6
six-fold primed rotation axis		6'

2.2.3 3-dimensional magnetic group symbols

Groups: Rod groups Layer groups 3-dimensional magnetic space groups

Table 2.2.3.1: Symmetry axes parallel to the plane of projection







Table 2.2.3.2: Symmetry axes normal to the plane of projection

Symmetry Axis or symmetry point	Graphical symbol	Screw vector of a right-handed screw rotation in units of the shortest non-primed translation vector parallel to the axis.	Printed symbol
Identity	None	None	1
Twofold unprimed rotation axis, 2		None	2





Tables			
Sixfold primed rotation axis, 6 primed	None	6'	
Sixfold unprimed screw axis, 6 sub 1	1/6	6 ₁	
Sixfold primed screw axis, 6 sub 1 primed	1/6	6 ₁ '	
Sixfold unprimed screw axis, 6 sub 2	1/3	6 ₂	
Sixfold primed screw axis, 6 sub 2 primed	1/3	6 ₂ '	
Sixfold unprimed screw axis, 6 sub 3	1/2	6 ₃	
Sixfold primed screw axis, 6 sub 3 primed	1/2	6 ₃ '	
Sixfold unprimed screw axis, 6 sub 4	2/3	64	
Sixfold primed screw axis, 6 sub 4 primed	2/3	64'	
Sixfold unprimed screw axis, 6 sub 5	5/6	6 ₅	

Sixfold primed screw axis, 6 sub 5 primed		5/6	6 ₅ '
Unprimed center of symmetry, unprimed inversion center, 1 bar	0	None	1
Primed center of symmetry, primed inversion center, 1 bar primed	•	None	1'
Twofold unprimed rotation axis with unprimed center of symmetry	•	None	2, 1 = 2/m
Twofold primed rotation axis with unprimed center of symmetry	•	None	2',1 = 2'/m'
Twofold unprimed rotation axis with primed center of symmetry	¢	None	2,ī' = 2/m'
Twofold primed rotation axis with primed center of symmetry	\diamond	None	2',1' = 2'/m
Twofold unprimed screw axis with unprimed center of symmetry	9	1/2	2 ₁ , 1
Twofold primed screw axis with unprimed center of symmetry	9	1/2	21',1

Tables			
Twofold unprimed screw axis with primed center of symmetry		2 ₁ ,1'	
Twofold primed screw axis with primed center of symmetry	1/2	2 ₁ ', <u>1</u> '	
Twofold primed screw axis with unprimed twofold rotation axis	1/2	21',2	
Twofold unprimed screw axis with primed twofold rotation axis	1/2	2 ₁ ,2'	
Twofold primed screw axis, twofold unprimed rotation axis, and primed and unprimed centers of symmetry	9 1/2	2 ₁ ',2,1,1'	
Twofold unprimed screw axis, twofold primed rotation axis, and primed and unprimed centers of symmetry	9 1/2	2 ₁ ,2',1',1	
Twofold primed rotation axis with center of symmetry Twofold screw axis with center of symmetry	ý 1/2	2',2 ₁ ,1	
Twofold rotation axis with center of symmetry, Two fold primed screw axis with center of symmetry	ý 1/2	2,2 ₁ ',1	
Threefold unprimed rotation axis with unprimed center of symmetry, inversion axis 3 bar	N one	3, 1 = 3	

Threefold unprimed rotation axis with primed center of symmetry, inversion axis 3 bar prime	None	3,1' = 3'
Threefold unprimed rotation axis with primed and unprimed centers of symmetry	None	3,1',1
Fourfold unprimed rotation axis with unprimed center of symmetry	None	4, 1 = 4/m
Fourfold primed rotation axis with unprimed center of symmetry	None	4',1 = 4'/m
Fourfold unprimed rotation axis with primed center of symmetry	None	4,1' = 4/m '
Fourfold primed rotation axis with primed center of symmetry	None	4',1' = 4'/m '
Fourfold unprimed screw axis with unprimed center of symmetry	1/2	4 ₂ ,1
Fourfold primed screw axis with unprimed center of symmetry	1/2	4 ₂ ', 1
Fourfold unprimed screw axis with primed center of symmetry	1/2	4 ₂ , <u>1</u> '



Tables			
Primed and unprimed inversion axes 4 bar and 4 bar prime, and primed twofold screw axis	1/2	4 4	
Sixfold unprimed rotation axis with unprimed center of symmetry	None	6, 1 = 6/m	
Sixfold primed rotation axis with unprimed center of symmetry	None	6',1 = 6'/m	
Sixfold unprimed rotation axis with primed center of symmetry	None	6,1' = 6/m'	
Sixfold primed rotation axis with primed center of symmetry	None	6',1' = 6'/m'	
Sixfold unprimed screw axis 6 sub 3 with unprimed center of symmetry	1/2	6 ₃ ,1	
Sixfold primed screw axis 6 sub 3 prime with unprimed center of symmetry	1/2	6 ₃ ', T	
Sixfold unprimed screw axis 6 sub 3 with primed center of symmetry	1/2	6 ₃ , T '	
Sixfold primed screw axis 6 sub 3 prime with primed center of symmetry	1/2	6 ₃ ', 1 '	

Sixfold unprimed rotation axis, sixfold primed screw axis 6 sub 3 prime	1/2	6 ₃ ', 6
Sixfold primed rotation axis, sixfold unprimed screw axis 6 sub 3	1/2	6 ₃ , 6'
Sixfold unprimed rotation axis, sixfold primed screw axis 6 sub 3 prime, with primed and unprimed centers of symmetry	1/2	6 ₃ ', 6 1,1'
Sixfold primed rotation axis, sixfold unprimed screw axis 6 sub 3, with primed and unprimed centers of symmetry	1/2	6₃', 6 1,1'
Unprimed inversion axis 6 bar	None	6
Primed inversion axis 6 bar prime	None	6'
Primed and unprimed inversion axes, 6 bar prime and 6 bar	None	<u>6</u> ', <u>6</u>
Primed and unprimed O	None	1',1

Table 2.2.3.3: Symmetry planes normal to the plane of projection

Symmetry plane	Graphical symbol	Glide vector in units of unprimed lattice translation parallel and normal to the projection plane	Printed symbol
Unprimed reflection plane		None	m
Primed reflection plane		None	m'
Unprimed axial glide plane		¹ ⁄ ₂ along line parallel to projection plane	a,b
Primed axial glide plane		¹ ⁄ ₂ along line parallel to projection plane	a',b'
Unprimed axial glide plane	••••	1/2 along line normal to projection plane	С
Primed axial glide plane	••••	¹ ⁄ ₂ along line normal to projection plane	с'
Unprimed diagonal glide plane		One glide plane with two components: ½ along line parallel to projection plane and ½ normal to projection plane	n
Primed diagonal glide plane	- • - • - • - • -	One glide plane with two components: ½ along line parallel to projection plane and ½ normal to projection plane	n'

Unprimed diamond glide plane		One glide plane with two components: 1/4 along line parallel to projection plane in dire and 1/4 up normal to projection p	d ection of arrow lane
Primed diamond glide plane		One glide plane with two components: 1/4 along line parallel to projection plane in dire and 1/4 up normal to projection p	d' ection of arrow lane
Unprimed diamond glide plane	F • F • F • F • F 4 • 4 • 4 • 4 • 4	One glide plane with two components: 1/4 along line parallel to projection plane in dire <i>and</i> 3/4 up normal to projection p	d ection of arrow lane
Primed diamond glide plane	* • * • * • * • * 4 • 4 • 4 • 4 • 4	One glide plane with two components: 1/4 along line parallel to projection plane in dire and 3/4 up normal to projection p	d' ection of arrow lane
Unprimed axial glide planes		<i>Two</i> glide planes each with one component: ½ along line parallel to projection plane; ½ normal to projection plane	a,b; c
Primed axial glide planes		<i>Two</i> glide planes each with one component: ½ along line parallel to projection plane; ½ normal to projection plane	a,b; c
Unprimed axial glide plane and primed axial glide plane	- • • - • • - • •	<i>Two</i> glide planes each with one component: ½ along line parallel to projection plane; ½ normal to projection plane	a',b'; c
Unprimed axial glide plane and primed axial glide plane	- • • - • • - • •	<i>Two</i> glide planes each with one component: ½ along line parallel to projection plane; ½ normal to projection plane	a,b; c'





Unprimed double glide plane and unprimed diagonal glide plane	<i>Three</i> glide planes each with one component ½ along directions parallel to the three arr	a,b,n ows
Primed double glide plane and primed diagonal glide plane	<i>Three</i> glide planes each with one component ½ along directions parallel to the three arr	a',b',n' ows
Unprimed double diagonal glide planes	Two glide planes each with one component ½ along directions parallel to the two arrow	d ws
Primed double diagonal glide planes	Two glide planes each with one component ½ along directions parallel to the two arrow	d' ws

Table 2.2.3.5: Symmetry axes inclined to the plane of projection (in cubic magnetic space groups only)

Symmetry plane	Graphical symbol	Screw vector of a right- handed screw rotation in units of the shortest unprimed lattice translation parallel to the axis	Printed symbol
Unprimed twofold rotation axis parallel to a face diagonal of the cube	·¢\$	None ⊸●	2
Primed twofold rotation axis parallel to a face diagonal of the cube	• 🖨 🚽	None ⊸●	2'
Unprimed twofold screw axis 2 sub 1 parallel to a face diagonal of the cube	•	/₂ -●	2 ₁

Primed twofold screw axis 2 sub 1 prime parallel to a face diagonal of the cube

Unprimed threefold rotation axis parallel to a body diagonal of the cube

Unprimed threefold screw axis 3 sub 1 parallel to a body diagonal of the cube

Primed threefold screw axis 3 sub 1prime parallel to a body diagonal of the cube

Unprimed threefold screw axis 3 sub 2 parallel to a body diagonal of the cube

Primed threefold screw axis 3 sub 2 prime parallel to a body diagonal of the cube

Unprimed inversion axis 3 bar parallel to a body diagonal of the cube

• • •	1/2	2 ₁ '
	None	3
	1/3	3 ₁
	1/3	3 ₁ '
	2/3	3 ₂
	2/3	3 ₂ '
	None	3,1 = 3

Table 2.2.3.6: Symmetry planes inclined to the plane of projection (in cubic magnetic space groups only)

Symmetry Plane Symbol	Graphical symbol for planes normal to		Glide vectors in units of unprimed lattice translation for planes normal to		Print
	[011] and [011];[1	101] and [10 <u>1</u>]	[011] and [011];[101] and [10 <u>1</u>]	
Unprimed Reflection plane		\bigcirc	None	None	m
Primed Reflection plane			None	None	m'
Unprimed axial glide plane		· · · · · · · · · · · · · · · · · · ·	½ along [100]	½ along [010]	a,b
Primed axial glide plane			½ along [100]	½ along [010]	a',b'
Unprimed axial glide plane			½ along [011] or [011]	½ along [10 <u>1</u>] or [101]	
Unprimed axial glide plane			½ along [011] or [011]	½ along [101] or [101]	



n





d'



Table 2.2.3.7: Height of symmetry operations above plane of projection

Heights are given as a fraction of the shortest primed or unprimed translation perpendicular to the plane of projection. Fractions are color coded black and red corresponding to related unprimed and primed operations, respectively. Examples are as follows:

Table 2.2.3.7a: Rotation axes, screw axes, inversion axes and reflection and glide planes parallel to the plane of projection



Table 2.2.3.7b: Inversion centers and inversion axes perpendicular to the plane of projection (i.e. height of inversion center of rotation-inversion)






Table

Table 2.3: Sets of three-dimensional magnetic space groups \mathbf{M}_{R} where the choice of \mathbf{t}_{α} in Tables 1.1 has led to identical Symmetry operations in the Tables of Properties of Magnetic Groups.

3.4.11	P _{2a} 2	49.10.373	P _{2a} ccm'
3.6.13	P _c 2	49.13.376	P _C ccm'
6.4.28	P _{2a} m	51.10.396	P _{2b} mma
6.6.30	P _c m	51.12.398	P _A mma
7.4.35	P _{2a} c	51.13.399	P _{2b} m'ma
7.6.37	P _c c	51.19.405	P _A m'ma
10.6.54	$P_{2a} 2/m$	75.5.665	P _P 4
10.8.56	$P_{c} 2/m$	75.6.666	P ₁ 4
13.6.82	$P_{2a} 2/c$	77.5.676	$P_P 4_2$
13.8.84	$P_{c} 2/c$	77.6.677	$P_1 4_2$
16.4.102 16.5.103 16.6.104	P _{2a} 222 P _c 222 P 222	81.5.697 81.6.698	P _P 4 P ₁ 4
17.5.110	$P_{2a} 222_{1}$	83.7.709	P _P 4/m
17.6.111	$P_{c} 222_{1}$	83.8.710	P _I 4/m
25.6.160 25.7.161 25.9.163	P₂a mm2 P _c mm2 P₅ mm2	89.7.753 89.8.754	P _P 422 P ₁ 422
26.6.173	$P_{2a}mc2_1$	99.7.829	P _P 4mm
26.8.175	$P_{c}mc2_1$	99.8.830	P _I 4mm
27.5.182	$P_{2a} cc2$	111.7.917	P _P 42m
27.6.183	$P_{c} cc2$	111.8.918	P₁42m
28.6.190	P _{2b} ma2	111.10.920	P _P 4'2m'
28.8.192	P ₄ ma2	111.11.921	P _I 4'2m'
47.6.352	P _{2a} mmm	115.7.947	P _P 4m2
47.7.353	P ₂ mmm	115.8.948	P₁4m2
47.8.354	P _F mmm	123.11.1009 123.12.1010	P _P 4/mmm P ₁ 4/mmm
47.9.355 47.11.357	P _{2a} mmm' P _c mmm'		
49.8.371 49.9.372	P _{2a} ccm P _c ccm		