

Tables of properties of magnetic subperiodic groups

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Tables of crystallographic properties of the magnetic subperiodic groups, *i.e.* the 31 magnetic frieze-group types, the 394 magnetic rod-group types and the 528 magnetic layer-group types are presented. The content and format is similar to that of non-magnetic subperiodic groups and space groups given in *International Tables for Crystallography*. Additional content for each group type includes a diagram of general positions with corresponding general magnetic moments, Seitz notation used as a second notation for symmetry operations, and general and special positions listed with the components of the corresponding magnetic moments allowed by symmetry.

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The magnetic frieze groups were first derived by Belov (1956) and the magnetic rod and layer groups by Neronova & Belov (1961) [see also the review by Zamorzaev & Palistrant (1980) and the monograph by Zamorzaev (1976)]. The magnetic subperiodic groups were rederived by Litvin (1999) as an extension of the non-magnetic subperiodic groups (Volume E of *International Tables for Crystallography*, 2002*b*). The form and meaning of the symbols used were in analogy to the form and meaning of the Opechowski–Guccione symbols (Opechowski & Guccione, 1965) for magnetic space groups, which differ (see Opechowski & Litvin, 1977) from the form and meaning of the symbols used by Belov (1956) and Neronova & Belov (1961).

We have compiled an electronic book entitled *Magnetic Subperiodic Groups*.¹ This book presents tables of crystallographic properties of the magnetic subperiodic groups with an extensive introduction and tables of equi-translational (*translationengleiche*) subgroups of the magnetic subperiodic groups. Also included is the survey of magnetic subperiodic groups (Litvin, 1999) listing the elements of these groups in Seitz notation.

An example of the tables of crystallographic properties, the table of crystallographic properties of the magnetic layer group $p_p\bar{4}2m$, is shown in Fig. 1. The content and format of these tables, *i.e.*

Headline

Diagrams of symmetry elements and general positions

Origin

Asymmetric unit

Symmetry operations

Generators selected

General and special positions

Symmetry of special projections,

is similar to the content and format of the crystallographic tables of the non-magnetic subperiodic groups and non-magnetic space groups presented in Volume E of *International Tables for Crystallography*

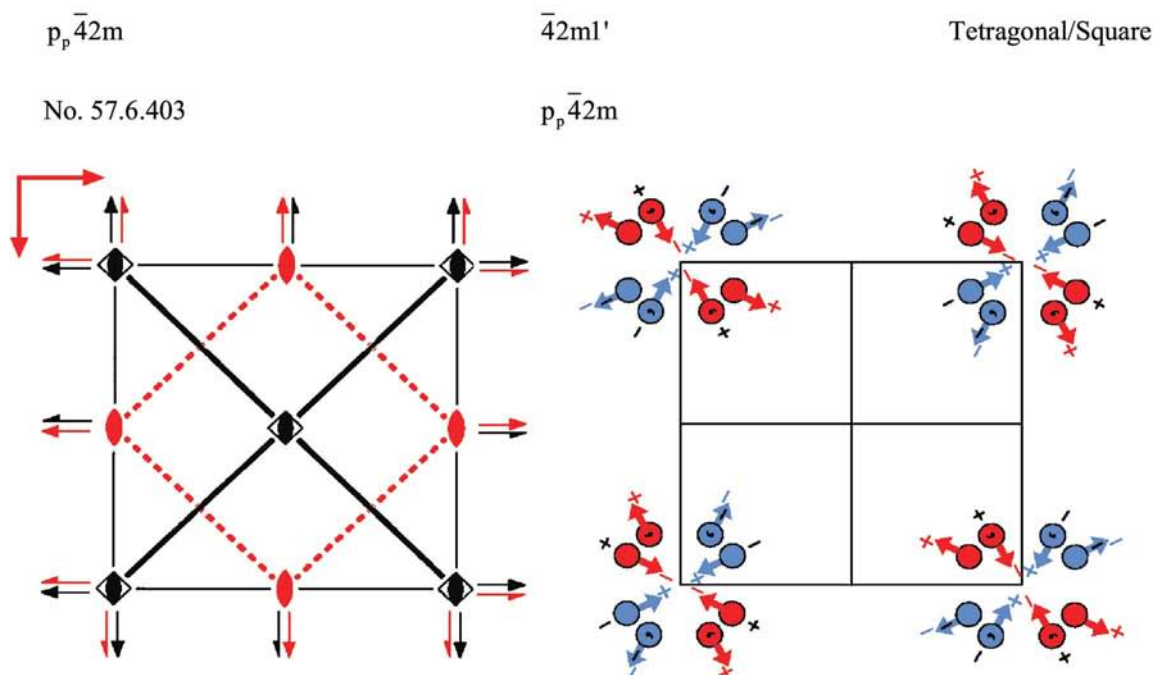
(2002*b*) and Volume A of *International Tables for Crystallography* (2002*a*), respectively.

While the content and format are similar, there are some distinct differences. In the diagrams of symmetry elements, on the upper left in Fig. 1, the symmetry elements are color coded: black symbols denote symmetry elements that are not coupled with time inversion, *e.g.* the unprimed mirror plane m_x, \bar{x}, z , which is denoted by a diagonal solid black line; red symbols denote symmetry elements that are coupled with time inversion, *e.g.* the primed glide plane $g'(\frac{1}{2}, \frac{1}{2}, 0)x + \frac{1}{2}, x, z$, the prime denoting that the glide-plane operation $g(\frac{1}{2}, \frac{1}{2}, 0)x + \frac{1}{2}, x, z$ is coupled with time inversion I' , which is denoted by a diagonal dashed red line. The translational subgroup of the magnetic layer group $p_p\bar{4}2m$ is denoted in the group symbol by p_p and by the two red arrows in the upper left corner of the symmetry diagram. Both denote that the translational subgroup is generated by the two translations $t'(1, 0, 0)$ and $t'(0, 1, 0)$, both translations coupled with time inversion.

In the general position diagram, the corresponding general magnetic moment at each position is indicated by an attached arrow. The black plus and minus signs indicate if the general position is above or below, respectively, the plane of the diagram. Each black plus and minus sign is in the same plane as the associated position. The height of each position is also coded into the color of the positions and arrows: red indicates that a position is above and blue that it is below the plane of the diagram. The colored plus and minus signs indicate if the associated arrow is tilted upward or downward relative to the plane of the diagram. A colored arrow tilted upward may obscure a black plus or minus sign associated with its position, *e.g.* each tilted up red arrow in Fig. 1 obscures an underlying black plus sign. This color coding of the general positions and associated magnetic moments is the same as that used in the three-dimensional general position VRML diagrams published by Cordisco & Litvin (2004).

In the listing of the symmetry operations, the Seitz notation is given below each operation. For example, below the notation for the mirror plane m_x, \bar{x}, z is the Seitz notation $(m_{xy}|0, 0, 0)$ and below the primed glide plane $g'(\frac{1}{2}, \frac{1}{2}, 0)x + \frac{1}{2}, x, z$ is $(m_{xy}|1, 0, 0)'$, the prime denoting that the glide plane $(m_{xy}|1, 0, 0)$ is coupled with time inversion I' . In the listing of general and special positions, after the coordinates of each

¹ The complete set of files that constitute this electronic book is available from the IUCr electronic archives (Reference: SH5024). Services for accessing these data are described at the back of the journal. These files may also be downloaded from <http://www.bk.psu.edu/faculty/Litvin> and are also available on CD on request from the author at u3c@psu.edu.



Origin at $\bar{4}2m$

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

Symmetry operations

For $(0,0,0)$ + set

- | | | | |
|--|--|---|--|
| (1) 1
(1 0,0,0) | (2) 2 $0,0,z$
(2 _z 0,0,0) | (3) $\bar{4}^+$ $0,0,z; 0,0,0$
($\bar{4}_z$ 0,0,0) | (4) $\bar{4}^-$ $0,0,z; 0,0,0$
($\bar{4}_z^{-1}$ 0,0,0) |
| (5) 2 $0,y,0$
(2 _y 0,0,0) | (6) 2 $x,0,0$
(2 _x 0,0,0) | (7) m x,\bar{x},z
(m _{xy} 0,0,0) | (8) m x,x,z
(m _{xy} ⁻ 0,0,0) |

For $(1,0,0)'$ + set

- | | | | |
|--|--|--|---|
| (1) t' $(1,0,0)$
(1 1,0,0)' | (2) 2' $\frac{1}{2},0,z$
(2 _z 1,0,0)' | (3) $\bar{4}^+$ $\frac{1}{2},\frac{1}{2},z; \frac{1}{2},\frac{1}{2},0$
($\bar{4}_z$ 1,0,0)' | (4) $\bar{4}^-$ $\frac{1}{2},\frac{1}{2},z; \frac{1}{2},\frac{1}{2},0$
($\bar{4}_z^{-1}$ 1,0,0)' |
| (5) 2' $\frac{1}{2},y,0$
(2 _y 1,0,0)' | (6) 2' $(1,0,0) \ x,0,0$
(2 _x 1,0,0)' | (7) g' $(\frac{1}{2},-\frac{1}{2},0) \ x + \frac{1}{2},\bar{x},z$
(m _{xy} 1,0,0)' | (8) g' $(\frac{1}{2},\frac{1}{2},0) \ x + \frac{1}{2},x,z$
(m _{xy} ⁻ 1,0,0)' |

Figure 1
Example table of crystallographic properties of a magnetic layer group.

short communications

Generators selected (1); $t'(1,0,0)$; $t'(0,1,0)$; (2); (3); (5)

Positions

		Coordinates			
Multiplicity, Wyckoff letter, Site Symmetry		(0,0,0) +	(1,0,0)' +		
8 j 1	(1) $x,y,z [u,v,w]$	(2) $\bar{x},\bar{y},z [\bar{u},\bar{v},w]$	(3) $y,\bar{x},\bar{z} [\bar{v},u,w]$	(4) $\bar{y},x,\bar{z} [v,\bar{u},w]$	
	(5) $\bar{x},y,\bar{z} [\bar{u},v,\bar{w}]$	(6) $x,\bar{y},\bar{z} [u,\bar{v},\bar{w}]$	(7) $\bar{y},\bar{x},z [v,u,\bar{w}]$	(8) $y,x,z [v,\bar{u},\bar{w}]$	
4 i ..m	$x,x,z [\bar{u},u,0]$	$\bar{x},\bar{x},z [u,\bar{u},0]$	$x,\bar{x},z [\bar{u},\bar{u},0]$	$\bar{x},x,\bar{z} [u,u,0]$	
4 h 2'..	$0,\frac{1}{2},z [u,v,0]$	$\frac{1}{2},0,\bar{z} [\bar{v},u,0]$	$0,\frac{1}{2},\bar{z} [\bar{u},v,0]$	$\frac{1}{2},0,z [\bar{v},\bar{u},0]$	
4 g .2'	$x,\frac{1}{2},0 [0,v,w]$	$\bar{x},\frac{1}{2},0 [0,v,\bar{w}]$	$\frac{1}{2},\bar{x},0 [\bar{v},0,w]$	$\frac{1}{2},x,0 [\bar{v},0,\bar{w}]$	
4 f .2.	$x,0,0 [u,0,0]$	$\bar{x},0,0 [\bar{u},0,0]$	$0,\bar{x},0 [0,u,0]$	$0,x,0 [0,\bar{u},0]$	
2 e 2.mm	$\frac{1}{2},\frac{1}{2},z [0,0,0]$	$\frac{1}{2},\frac{1}{2},\bar{z} [0,0,0]$			
2 d 2.mm	$0,0,z [0,0,0]$	$0,0,\bar{z} [0,0,0]$			
2 c 2'22'	$\frac{1}{2},0,0 [u,0,0]$	$0,\frac{1}{2},0 [0,\bar{u},0]$			
1 b $\bar{4}'2'm$	$\frac{1}{2},\frac{1}{2},0 [0,0,0]$				
1 a $\bar{4}2m$	$0,0,0 [0,0,0]$				

Symmetry of special projections

Along [001] p_p4mm
 $\mathbf{a}^* = \mathbf{a}$ $\mathbf{b}^* = \mathbf{b}$
 Origin at $\frac{1}{2},\frac{1}{2},z$

Along [100] $p_a2m'm'$
 $\mathbf{a}^* = \mathbf{b}$
 Origin at $x,0,0$

Along [110] $p1m11'$
 $\mathbf{a}^* = (-\mathbf{a}+\mathbf{b})/2$
 Origin at $x,x,0$

Figure 1 (continued)

Table 1
Equi-translational subgroups of the magnetic layer group $p_p\bar{4}2m$.

$p_p\bar{4}2m$		$p\bar{4}m2$	(000; a−b, a+b, c)	(1 000)	($\bar{4}_z$ 000)	(2_z 000)	($\bar{4}_z^{-1}$ 000)
$p_p\bar{4}$	(000; a, b, c)	$p\bar{4}$	(000; a−b, a+b, c)	(1 000)	($\bar{4}_z$ 000)	(m_{xy} 000)	(m_{xy} 000)
p_c222	(000; a, b, c)	$c222$	(000; 2a, 2b, c)	(1 000)	($\bar{4}_z$ 000)	(2_z 000)	($\bar{4}_z^{-1}$ 000)
c_pmm2	(000; a−b, a+b, c)	$pmm2$	(000; a−b, a+b, c)	(1 000)	(2_x 000)	(2_y 000)	(2_z 000)
p_c211	(000; a, b, c)	$c211$	(000; 2a, 2b, c)	(1 000)	(m_{xy} 000)	(m_{xy} 000)	(2_z 000)
p_c211	(000; b, \bar{a} , c)	$c211$	(000; 2b, $2\bar{a}$, c)	(1 000)	(2_x 000)	(2_y 000)	(2_z 000)
$p_{2a}112$	(000; a, a+b, c)	$p112$	(000; 2a, a+b, c)	(1 000)	(2_x 000)	(2_y 000)	(2_z 000)
$c_p m11$	(000; a+b, −a+b, c)	$pm11$	(000; a+b, −a+b, c)	(1 000)	(2_x 000)	(2_y 000)	(2_z 000)
$c_p m11$	(000; a−b, a+b, c)	$pm11$	(000; a−b, a+b, c)	(1 000)	(m_{xy} 000)	(m_{xy} 000)	(m_{xy} 000)
$p_{2a}1$	(000; a, a+b, c)	$p1$	(000; 2a, a+b, c)	(1 000)	(m_{xy} 000)	(m_{xy} 000)	(m_{xy} 000)

position, the components of the symmetry-allowed magnetic moment at that position are given within square brackets. For example, in the set of special positions denoted by the Wyckoff letter g, with site symmetry $.2'$, the first entry in the row is $x, \frac{1}{2}, 0 [0, v, w]$. This means that at position $x, \frac{1}{2}, 0$, whose site symmetry consists of the identity and a twofold primed rotation about the x axis, the symmetry-allowed magnetic moment is in the direction $[0, v, w]$.

As an example of the tables of equi-translational subgroups of the magnetic subperiodic groups, in Table 1 we give the table of equi-translational subgroups of the magnetic layer group $p_p\bar{4}2m$. This group is listed in the first row and its equi-translational subgroups in the following rows. Each equi-translational subgroup is defined by the translational group of $p_p\bar{4}2m$ and the elements of $p_p\bar{4}2m$ listed on the extreme right hand side. The second column gives the coordinate system, *i.e.* origin and conventional basis vectors, of the subgroup in terms of the coordinate system of the group $p_p\bar{4}2m$. The third and fourth columns give the symbol and coordinate system of the non-magnetic subgroup of index two of each group. For example, the equi-translational subgroup $p_p\bar{4}$ is defined by the translational group p_p and the elements (1|000), ($\bar{4}_z$ |000), (2_z |000) and ($\bar{4}_z^{-1}$ |000) in the same coordinate system as the group $p_p\bar{4}2m$. The subgroup $p\bar{4}$ of elements not coupled with time inversion is defined by a translational group denoted by p and the four elements given to the right in the conventional coordinate system (000; a−b, a+b, c). The coordinate

system implies that the translational group p of $p\bar{4}$ is generated by the translations $t(\bar{1}10)$ and $t(110)$.

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