International Tables for Crystallography (2016). Vol. A, Section 3.6.2.2.5, pp. 856–857.

The impact of this convention is that nine Opechowski–Guccione symbols of three-dimensional magnetic space groups need to be changed:

	Old symbol	New symbol
93.6.781	$P_{2c}4_222$	$P_{2c}4_222'$
93.8.783	P_I4_222	P_I4_222'
93.9.784	$P_{2c}4_2'22'$	$P_{2c}4_2'22$
153.4.1270	$P_{2c}3_112$	$P_{2c}3_112'$
154.4.1274	$P_{2c}3_121$	$P_{2c}3_12'1$
180.6.1401	$P_{2c}6_222$	$P_{2c}6_222'$
180.7.1402	$P_{2c}6_2'22'$	$P_{2c}6_2'22$
181.6.1408	$P_{2c}6_422$	$P_{2c}6_422'$
181.7.1409	$P_{2c}6_4'2'2$	$P_{2c}6_4'2'2'$

To have all $\mathcal{M}_R$ group symbols represent subgroups $\mathcal{D}$, six symbols for three-dimensional magnetic space groups were based (Opechowski & Guccione, 1965) on the symbol of the subgroup $\mathcal{D}$ instead of the symbol for $\mathcal{F}$. These are the groups 144.3.1236 $P_{2c}3_2$, 145.3.1239 $P_{2c}3_1$, 151.4.1262 $P_{2c}3_212$, 152.4.1266 $P_{2c}3_221$, 153.4.1270 $P_{2c}3_112$ and 154.4.1274 $P_{2c}3_121$. Additional groups are the rod groups 43.3.231 $\not{p}_{2c}3_2$, 44.3.234 $\not{p}_{2c}3_1$, 47.4.246 $\not{p}_{2c}3_212$ and 48.4.250 $\not{p}_{2c}3_112$.

3.6.2.2.5. *Symbol of the subgroup $\mathcal{D}$ of index 2 of $\mathcal{F}(\mathcal{D})$*

For magnetic group types $\mathcal{F}(\mathcal{D})$, the magnetic group type symbol of the subgroup $\mathcal{D}$ is given in the third column of the survey of magnetic groups, see *e.g.* Table 3.6.2.2. If $\mathcal{F}(\mathcal{D})$ is a group $\mathcal{M}_T$, then the subgroup $\mathcal{D}$ is defined by the translational group of $\mathcal{F}(\mathcal{D})$ and the unprimed coset representatives of $\mathcal{F}(\mathcal{D})$.

Example

Consider the three-dimensional magnetic space-group type 16.3.101 $P2'2'2$. The representative group $P2'2'2$ is defined by the translational subgroup $\mathcal{T}$ denoted by the letter P generated by the translations

$$\{1|1,0,0)\}\quad \{1|0,1,0\}\quad \{1|0,0,1\}$$

and the standard set of coset representatives

$$\{1|0\}\quad \{2_{100}|0\}'\quad \{2_{010}|0\}'\quad \{2_{001}|0\}.$$

The subgroup $\mathcal{D}$ of index 2 of the representative group $\mathcal{F}(\mathcal{D}) = P2'2'2$ is defined by the translational group $\mathcal{T}$ denoted by the letter P and the cosets $\{1|0\}$ and $\{2_{001}|0\}$, and is a group of type $P2$.

If $\mathcal{F}(\mathcal{D})$ is a group $\mathcal{M}_R$, then the subgroup $\mathcal{D}$ is defined by the non-primed translational group of $\mathcal{F}(\mathcal{D})$ and all the cosets of the standard set of coset representatives of the group $\mathcal{F}(\mathcal{D})$.

Example

Consider the three-dimensional magnetic space-group type 16.4.102 $P_{2a}222$. The representative group $P_{2a}222$ is defined by the translational group $\mathcal{T}$ denoted by the symbol P_{2a} generated by the translations

$$\{1|1,0,0\}'\quad \{1|0,1,0\}\quad \{1|0,0,1\}$$

and the standard set of coset representatives

$$\{1|0\}\quad \{2_{100}|0\}\quad \{2_{010}|0\}\quad \{2_{001}|0\}.$$

The subgroup $\mathcal{D}$ of index 2 of the representative group $\mathcal{F}(\mathcal{D}) = P_{2a}222$ is defined by the translational subgroup $\mathcal{T}$ denoted by the symbol P_{2a}, *i.e.* the translations generated by

$$\{1|2,0,0\}\quad \{1|0,1,0\}\quad \{1|0,0,1\}$$

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

While the group type symbol of $\mathcal{D}$ is given, the coset representatives of the subgroup $\mathcal{D}$ of $\mathcal{F}(\mathcal{D})$ derived from the standard set of coset representatives of $\mathcal{F}(\mathcal{D})$ may not be identical with the standard set of coset representatives of the representative group of type $\mathcal{D}$ found in the survey of magnetic group types. Consequently, to show the relationship between this subgroup $\mathcal{D}$ and the listed representative group of groups of type $\mathcal{D}$ additional information is provided: a new coordinate system is defined in which the coset representatives of this subgroup $\mathcal{D}$ are identical with the standard set of coset representatives listed for the representative group of groups of type $\mathcal{D}$: Let (O; **a**, **b**, **c**) be the coordinate system in which the group $\mathcal{F}(\mathcal{D})$ 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 centred lattices. A second coordinate system, defined by (O + **p**; **a**′, **b**′, **c**′), is given in which the coset representatives of this subgroup $\mathcal{D}$ are identical with the standard set of coset representatives listed for the representative group of groups of type $\mathcal{D}$. O + **p** is referred to as the *location* of the subgroup $\mathcal{D}$ in the coordinate system of the group $\mathcal{F}(\mathcal{D})$ (Kopský, 2011). The origin is first translated from O to O + **p**. On translating the origin from O to O + **p**, a coset representative $\{\boldsymbol{R}|\boldsymbol{\tau}\}$ becomes $\{\boldsymbol{R}|\boldsymbol{\tau} + \boldsymbol{Rp} - \boldsymbol{p}\}$ (Litvin, 2005, 2008*b*; see also Section 1.5.2.3). This is followed by changing the basis vectors **a**, **b** and **c** to **a**′, **b**′ and **c**′, respectively. The basis vectors **a**′, **b**′, **c**′ define the conventional unit cell of the non-primed subgroup $\mathcal{D}$ of $\mathcal{F}(\mathcal{D})$ in the coordinate system (O; **a**, **b**, **c**) in which $\mathcal{F}(\mathcal{D})$ is defined. (O + **p**; **a**′, **b**′, **c**′) is given immediately following the group type symbol for the subgroup $\mathcal{D}$ of $\mathcal{F}(\mathcal{D})$. [In Litvin (2013), for typographical simplicity, the symbols 'O +' are omitted.]

Example

For the three-dimensional magnetic space-group type 10.4.52, $\mathcal{F}(\mathcal{D}) = P2/m'$, one finds in Litvin (2013)[2]

Serial No.	Symbol	Non-primed subgroup of index 2	Standard set of coset representatives
10.4.52	$P2/m'$	$P2$ (0, 0, 0; **a**, **b**, **c**)	$\{1|0\}$ $\{2_{010}|0\}$ $\{\bar{1}|0\}'$ $\{m_{010}|0\}'$

The translational subgroup of the subgroup $\mathcal{D} = P2$ of $\mathcal{F}(\mathcal{D}) = P2/m'$ 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 are $\{1|0\}$ and $\{2_{010}|0\}$, the unprimed coset representatives on the right. This subgroup $\mathcal{D}$ is of type $P2$. In Litvin (2013), 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.* $\mathbf{p} = (0,0,0)$ and $\mathbf{a}' = \mathbf{a}$, $\mathbf{b}' = \mathbf{b}$ and $\mathbf{c}' = \mathbf{c}$. In the coordinate system of the magnetic group $P2/m'$, the coset representatives of its subgroup $\mathcal{D} = P2$ are identical with the standard set of coset representatives of the group type $P2$.

[2] In Litvin (2013) the terminology 'non-magnetic' is used in place of 'non-primed' in the column headings in these tables.

Example

For the three-dimensional magnetic space-group type 16.7.105, $\mathcal{F}(\mathcal{D}) = P_{2c}22'2'$ one has

Serial No.	Symbol	Non-primed subgroup of index 2	Standard set of coset representatives
16.7.105	$P_{2c}22'2'$	$P222_1$ (0, 0, 0; **a**, **b**, 2**c**)	$\{1\|0\}$ $\{2_{100}\|0\}$ $\{2_{010}\|0, 0, 1\}$ $\{2_{001}\|0, 0, 1\}$

The translational subgroup of the subgroup $\mathcal{D} = P222_1$ of $\mathcal{F}(\mathcal{D}) = P_{2c}22'2'$ 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 $\mathcal{D}$ is of type $P222_1$. Listed for the group type 17.1.106 $P222_1$, one finds a different set of coset representatives:

$$\{1|0\} \quad \{2_{100}|0\} \quad \{2_{010}|0, 0, \tfrac{1}{2}\} \quad \{2_{001}|0, 0, \tfrac{1}{2}\}.$$

Consequently, to show the relationship between this subgroup $\mathcal{D}$ of $\mathcal{F}(\mathcal{D})$ and the listed representative group of the group type $P222_1$ we change the coordinate system in which $\mathcal{D}$ is defined to (0, 0, 0; **a**, **b**, 2**c**). In this new coordinate system the coset representatives of the subgroup $\mathcal{D}$ are identical with the coset representatives of the representative group of the group type $P222_1$.

Example

For the three-dimensional magnetic space-group type 18.4.116, $P2_12_1'2'$, one has

Serial No.	Symbol	Non-primed subgroup of index 2	Standard set of coset representatives
18.4.116	$P2_12_1'2'$	$P2_1$ (0, $\frac{1}{4}$, 0; **c**, **a**, **b**)	$\{1\|0\}$ $\{2_{100}\|\frac{1}{2}, \frac{1}{2}, 0\}$ $\{2_{010}\|\frac{1}{2}, \frac{1}{2}, 0\}'$ $\{2_{001}\|0\}'$

The translational subgroup of $\mathcal{D}$ 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 $\{1|0\}$ and $\{2_{100}|\frac{1}{2}, \frac{1}{2}, 0\}$, the unprimed coset representatives on the right. The group $\mathcal{D}$ is of type $P2_1$. For the magnetic group type 4.1.15 $P2_1$ one finds a different set of coset representatives: $\{1|0\}$ and $\{2_{010}|0, \frac{1}{2}, 0\}$. Consequently, to show the relationship between the subgroup $\mathcal{D}$ of $\mathcal{F}(\mathcal{D})$ and the listed representative group of the group type $P2_1$, we change the coordinate system in which the subgroup $\mathcal{D}$ is defined to (0, $\frac{1}{4}$, 0; **c**, **a**, **b**). The origin is first translated from O to $O + \mathbf{p}$, where $\mathbf{p} = (0, \frac{1}{4}, 0)$, and then a new set of basis vectors, $\mathbf{a}' = \mathbf{c}$, $\mathbf{b}' = \mathbf{a}$ and $\mathbf{c}' = \mathbf{b}$, is defined. In this new coordinate system the coset representatives of the subgroup $\mathcal{D}$ are identical with the standard set of coset representatives of the representative group of the group type $P2_1$.

3.6.3. Tables of properties of magnetic groups

In this section we present a guide to the tables of properties of the two- and three-dimensional magnetic subperiodic groups and the one-, two- and three-dimensional magnetic space groups given by Litvin (2013). The format and content of these magnetic group tables are similar to the format and content of the space-group tables in the present volume, the subperiodic group tables in *IT* E, and previous compilations of magnetic subperiodic groups (Litvin, 2005) and magnetic space groups (Litvin, 2008*b*). An example of one these tables is given in Fig. 3.6.3.1. The tables of properties of magnetic groups contain:

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

Tabulations of properties of three-dimensional magnetic space groups can also be found in Koptsik (1968) (note that the general-position diagrams are of 'black and white' objects, not spins). Neutron-diffraction extinctions can be found in the work of Ozerov (1969*a*,*b*) and on the Bilbao Crystallographic Server, http://www.cryst.ehu.es (Aroyo *et al.*, 2006). General positions and Wyckoff positions of the three-dimensional magnetic space groups can also be found on the Bilbao Crystallographic Server.

3.6.3.1. 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 3.6.3.3 below.) This lattice diagram depicts the coordinate system used, the conventional unit cell of the space group $\mathcal{F}$, the magnetic space group's magnetic superfamily type and the generators of the translational subgroup of the magnetic space group. In Fig. 3.6.3.2 we show lattice diagrams for two orthorhombic magnetic space groups: (*a*) $Pmc2_1$ and (*b*) $P_{2b}m'c'2_1$. The generating lattice vectors are colour coded. Those coloured black are not coupled with time inversion, while those coloured red are coupled with time inversion. In the group $Pmc2_1$, a magnetic group of the type $\mathcal{F}$, the lattice is an orthorhombic P lattice, see Fig. 3.6.3.2(*a*), and no generating translation is coupled with time inversion. In the second group, $P_{2b}m'c'2_1$, a magnetic group of type $\mathcal{M}_R$, the lattice is an orthorhombic P_{2b} lattice, see Fig. 3.6.3.2(*b*), and the generating lattice vector in the *y* direction is coupled with time inversion.

3.6.3.2. Heading

Each table begins with a headline consisting of two lines with five entries, for example

$P4/m'mm$	$4/m'mm$	Tetragonal
123.3.1001	$P4/m'2'/m2'/m$	

For three-dimensional magnetic space groups, this headline is to the right of the lattice diagram. 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 3.6.2.2), which belongs to this magnetic space-group

references