International Tables for Crystallography (2016). Vol. A, Section 3.6.3.2, pp. 857–858.

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.

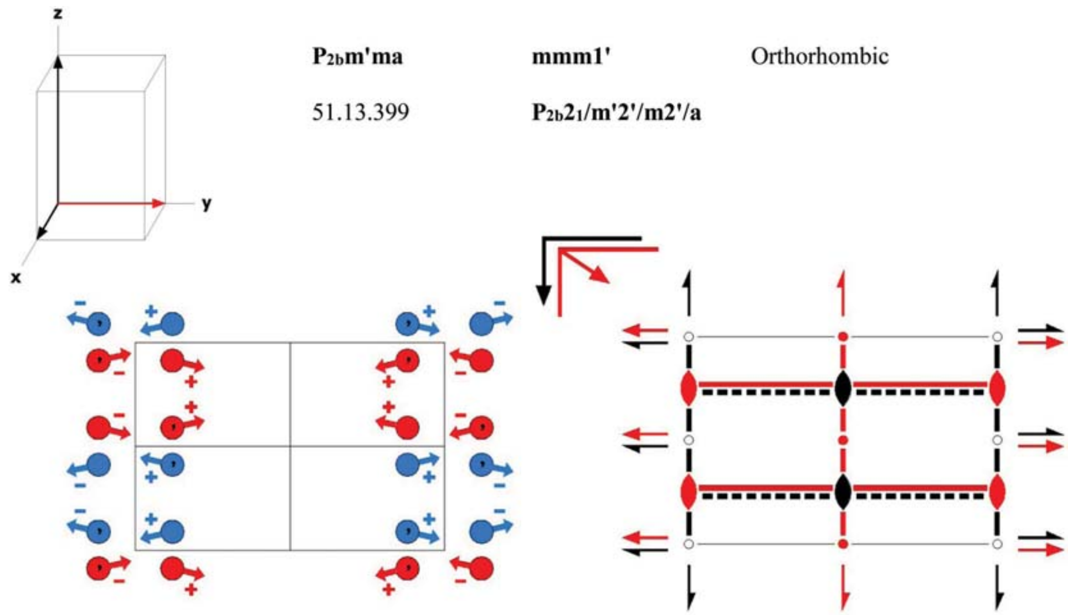
3.6.3.2. Heading

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



Origin at center (2'/m) at $2_1 2/ma$

Asymmetric unit $0 \le x \le 1/4$; $0 \le y \le 1/2$; $0 \le z \le 1$

Symmetry Operations

For (0,0,0) + set

(1) 1	(2) 2' ¼,0,z	(3) 2' 0,y,0	(4) 2 (½,0,0) x,0,0
$\{1 \mid 0\}$	$\{2_{001} \mid 1/2,0,0\}'$	$\{2_{010} \mid 0\}'$	$\{2_{100} \mid 1/2,0,0\}$
(5) $\bar{1}'$	(6) a (½,0,0) x,y,0	(7) m x,0,z	(8) m' ¼,y,z
$\{\bar{1} \mid 0\}'$	$\{m_{001} \mid 1/2,0,0\}$	$\{m_{010} \mid 0\}$	$\{m_{100} \mid 1/2,0,0\}'$

For (0,1,0)' + set

(2) t' (0,1,0)'	(2) 2 ¼,½,z	(3) 2 (0,1,0) 0,y,0	(4) 2' (½,0,0) x,½,0
$\{1 \mid 0,1,0\}'$	$\{2_{001} \mid 1/2,1,0\}$	$\{2_{010} \mid 0,1,0\}$	$\{2_{100} \mid 1/2,1,0\}'$
(5) $\bar{1}$ (0, ½,0)	(6) n' (½,1,0) x,y,0	(7) m' x,½,z	(8) b (0,1,0) ¼,y,z
$\{\bar{1} \mid 0,1,0\}$	$\{m_{001} \mid 1/2,1,0\}'$	$\{m_{010} \mid 0,1,0\}'$	$\{m_{100} \mid 1/2,1,0\}$

Figure 3.6.3.1
Table of properties of the three-dimensional magnetic space group 51.13.399 $P_{2b}m'ma$.

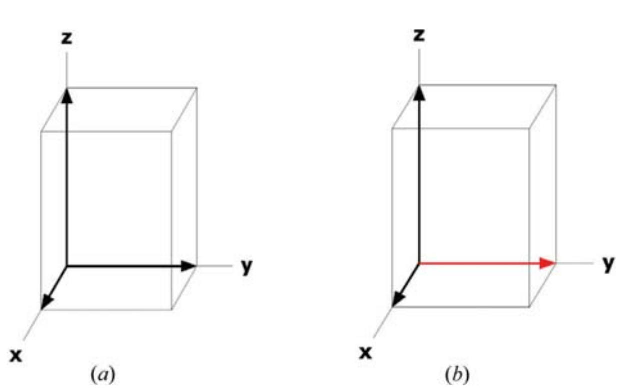


Figure 3.6.3.2
Lattice diagrams of (*a*) the three-dimensional magnetic space group 26.1.168 $\mathcal{F} = Pmc2_1$ and (*b*) the three-dimensional magnetic space group 26.10.177 $\mathcal{M}_R = P_{2b}m'c'2_1 = \mathcal{F}(\mathcal{D}) = Pmc2_1(Pca2_1)$.

type. Given a coordinate system, this group is defined by the list of symmetry operations (see Section 3.6.3.6) 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 3.6.3.9).

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

(3) The crystal system or crystal system/Bravais system classification 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 Section 3.6.2.2.1).

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