*International Tables for Crystallography* (2016). Vol. A, Section 3.6.2.2.4, pp. 854–856.



system. The absolute lengths of translation vectors, the position in space of the origin of the coordinate system and the orientation in that space of the basis vectors of that coordinate system are not explicitly given.

*3.6.2.2.3. Standard set of coset representatives*

The standard set of coset representatives of each representative group is listed on the right-hand side of the survey of magnetic group types, see *e.g.* Table 3.6.2.2. Each coset in the standard set of coset representatives is given in Seitz notation (Seitz, 1934, 1935*a*,*b*, 1936), *i.e.* $\{\boldsymbol{R}|\boldsymbol{\tau}\}$ or $\{\boldsymbol{R}|\boldsymbol{\tau}\}'$. $\boldsymbol{R}$ denotes a proper or improper rotation (rotation-inversion), $\boldsymbol{\tau}$ a non-primitive translation with respect to the non-primed translational subgroup of the magnetic group, and the prime denotes that $\{\boldsymbol{R}|\boldsymbol{\tau}\}$ is coupled with time inversion. The subindex notation on $\boldsymbol{R}$, denoting the orientation of the proper or improper rotation, is given in Table 1.4 of Litvin (2013). [Note that the Seitz notation used in Litvin (2013) predates and is different from the IUCr standard convention for Seitz symbolism, see Section 1.4.2.2 and Glazer *et al.* (2014).]

*3.6.2.2.4. Opechowski–Guccione magnetic group type symbols and the standard set of coset representatives*

The specification of the magnetic group type symbol and the standard set of coset representatives of the magnetic group type's representative group is based on the conventions introduced by Opechowski and Guccione (Opechowski & Guccione, 1965; Opechowski, 1986) for three-dimensional magnetic space groups. The specification was made in conjunction with Volume I of *International Tables for X-ray Crystallography* (1969) (abbreviated here as *ITXC* I). One finds in *ITXC* I, for each group type $\mathcal{F}$, a specification of the coordinate system used, and, in terms of that coordinate system, a specification of the subgroup of translations $\mathcal{T}$ of the representative space group of that group type, and also indirectly a specification of a set of coset representatives of $\mathcal{T}$ of that representative group of group type $\mathcal{F}$. These coset representatives are uniquely determined from the coordinate triplets of the explicitly printed general position of the space group. The symbol $\mathcal{F}$ for the space group is taken to be the space-group symbol at the top of the page listing these coordinate triplets. The symbol for a group type $\mathcal{F}1'$ is that of the group type $\mathcal{F}$ followed by $1'$, and the coset representatives of the representative group of the group type $\mathcal{F}1'$ consist of the set of coset representatives of $\mathcal{F}$ and this set multiplied by $1'$.

*Example*

In *ITXC* I, on the page for $\mathcal{F} = P2/m$ one finds the following coordinate triplets of the general position:

$$x, y, z; \quad x, y, \bar{z}; \quad \bar{x}, \bar{y}, z; \quad \bar{x}, \bar{y}, \bar{z}$$

determining the coset representative of the representative group $P2/m$:

$$\{1|0\}; \quad \{m_{001}|0\}; \quad \{2_{001}|0\}; \quad \{\bar{1}|0\}.$$

The coset representatives of the representative group $P2/m1'$ are then:

$$\begin{array}{llll} \{1|0\}; & \{m_{001}|0\}; & \{2_{001}|0\}; & \{\bar{1}|0\} \\ \{1|0\}'; & \{m_{001}|0\}'; & \{2_{001}|0\}'; & \{\bar{1}|0\}'. \end{array}$$

*ITXC* I has been replaced by *IT* A. Ones finds that, for some space groups, the set of coordinate triplets of the general positions explicitly printed in *IT* A differs from that explicitly printed in *ITXC* I. As a consequence, if one attempts to interpret the Opechowski–Guccione symbols (OG symbols) for magnetic groups using *IT* A, one will, in many cases misinterpret the meaning of the symbol (Litvin, 1997, 1998). [It was suggested in these two papers that the original set of OG symbols should be modified so one could correctly interpret them using *IT* A instead of *ITXC* I. Adopting this ill-advised suggestion would have required in the future a new modification of the OG symbols whenever changes were made to the choices of coordinate triplets of the general position in *IT* A. Consequently, the meaning of the original OG symbols was specified by Litvin (2001) by explicitly giving the coset representatives of the representative groups of each three-dimensional magnetic space group.]

*Magnetic groups $\mathcal{M}_T$*

The symbol for a magnetic group type $\mathcal{M}_T = \mathcal{F}(\mathcal{D}) = \mathcal{D} \cup (\mathcal{F} - \mathcal{D})1'$ and its representative group is based on the symbol for the group type $\mathcal{F}$. $\mathcal{D}$ is an equi-translational subgroup of $\mathcal{F}$, *i.e.* the translational subgroup $\mathcal{T}^{\mathcal{M}_T}$ of the magnetic group $\mathcal{M}_T$ is $\mathcal{T}$, the translational subgroup of $\mathcal{F}$. The translational part of the group type symbol of an $\mathcal{M}_T$ group is then the same as that of the group type $\mathcal{F}$. A number or letter in the remaining part of the symbol of $\mathcal{F}$ appears unchanged in the symbol for $\mathcal{M}_T$ if it is associated with a coset representative of the representative group $\mathcal{F}$ that is also an element contained in the subgroup $\mathcal{D}$ of $\mathcal{F}$. If not in $\mathcal{D}$, *i.e.* if in $\mathcal{F} - \mathcal{D}$, the number or letter appears in the symbol for $\mathcal{M}_T$ with a prime to denote that the element in $\mathcal{M}_T$ is coupled with $1'$.

*Example*

The orthorhombic space-group type $\mathcal{F} = Pca2_1$ has the magnetic space-group type number 29.1.198. The representative group is defined by a orthorhombic translational subgroup $\mathcal{T}$ denoted by the letter $P$ in $Pca2_1$ and the standard set of coset representatives

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

The magnetic space-group type 29.5.202 is a group $\mathcal{M}_T$ whose symbol is $Pc'a'2_1$. In this case we have $Pc'a'2_1 = P2_1 \cup (Pca2_1 - P2_1)1'$, *i.e.* $\mathcal{F} = Pca2_1$ and $\mathcal{D} = P2_1$. The symbol '$2_1$' in the symbol for $\mathcal{F} = Pca2_1$ refers to the coset representative $\{2_{001}|0, 0, \tfrac{1}{2}\}$, an element in $\mathcal{D} = P2_1$. Consequently, the symbol '$2_1$' appears unprimed in the symbol for $\mathcal{M}_T$ ($Pc'a'2_1$) and the coset representative $\{2_{001}|0, 0, \tfrac{1}{2}\}$ appears as an unprimed coset representative in the standard set of coset representatives of $\mathcal{M}_T$. The symbols '$c$' and '$a$' in $\mathcal{F} = Pca2_1$ refer to the coset representatives $\{m_{100}|\tfrac{1}{2}, 0, \tfrac{1}{2}\}$ and $\{m_{010}|\tfrac{1}{2}, 0, 0\}$, respectively, neither of which are contained in $\mathcal{D}$. Consequently, both symbols appear primed in the symbol $Pc'a'2_1$ for $\mathcal{M}_T$ and the coset representatives $\{m_{100}|\tfrac{1}{2}, 0, \tfrac{1}{2}\}$ and $\{m_{010}|\tfrac{1}{2}, 0, 0\}$ appear as primed coset representatives in the standard set of coset representatives of $\mathcal{M}_T$. The representative magnetic space group $Pc'a'2_1$ then has the orthorhombic translational subgroup $\mathcal{T}$ denoted by the letter $P$ and the standard set of coset representatives

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

*Magnetic groups $\mathcal{M}_R$*

The symbol for a group type $\mathcal{M}_R = \mathcal{F}(\mathcal{D}) = \mathcal{D} \cup (\mathcal{F} - \mathcal{D})1'$ and its representative group is also based on the symbol for the group $\mathcal{F}$. [This is in contradistinction to the BNS symbols of $\mathcal{M}_R$ groups (Belov *et al.*, 1957), where the symbol for an $\mathcal{M}_R$ group type is based on the symbol for the group $\mathcal{D}$, see Section 3.6.4.] As this is an equi-class magnetic group, half the translations of $\mathcal{F}$ are now coupled with $1'$ in $\mathcal{M}_R$ and half the translations remain unprimed in $\mathcal{M}_R$. The unprimed translations constitute the translational subgroup $\mathcal{T}^{\mathcal{D}}$ of $\mathcal{D}$. We can then write the coset decomposition of the translational subgroup $\mathcal{T}$ of $\mathcal{F}$ with respect to the translational subgroup $\mathcal{T}^{\mathcal{D}}$ of $\mathcal{D}$ as

$$\mathcal{T} = \mathcal{T}^{\mathcal{D}} \cup t_\alpha \mathcal{T}^{\mathcal{D}},$$

where $t_\alpha$ denotes a chosen coset representative, a translation of $\mathcal{F}$ which appears primed (coupled with $1'$) in $\mathcal{M}_R$. The translational subgroup $\mathcal{T}^{\mathcal{M}_R}$ of $\mathcal{M}_R$ can then be written as

$$\mathcal{T}^{\mathcal{M}_R} = \mathcal{T}^{\mathcal{D}} \cup t_\alpha{}' \mathcal{T}^{\mathcal{D}}.$$

Symbols for the translational groups $\mathcal{T}$, the translational subgroups $\mathcal{T}^{\mathcal{D}}$ of $\mathcal{T}$, the translational groups $\mathcal{T}^{\mathcal{M}_R}$ of $\mathcal{M}_R$ and the choice of the translations $t_\alpha$ are given in Fig. 1 of Litvin (2013).

The symbol for a magnetic group type $\mathcal{M}_R = \mathcal{F}(\mathcal{D})$ and its representative group is based on the symbol of the group type $\mathcal{F}$, and is also a symbol for the subgroup $\mathcal{D}$ of unprimed elements: the translational part of the symbol of $\mathcal{F}$ is replaced by the symbol for the translational subgroup $\mathcal{T}^{\mathcal{D}}$ of $\mathcal{D}$. If a coset representative $\{\boldsymbol{R}|\boldsymbol{\tau}(\boldsymbol{R})\}$ of $\mathcal{T}$ in $\mathcal{F}$ appears as the coset representative $\{\boldsymbol{R}|\boldsymbol{\tau}(\boldsymbol{R}) + \boldsymbol{t}_\alpha\}$ of $\mathcal{T}^{\mathcal{D}}$ in $\mathcal{D}$, then the number or letter corresponding to $\{\boldsymbol{R}|\boldsymbol{\tau}(\boldsymbol{R})\}$ in the symbol for $\mathcal{F}$ is primed. If $\{\boldsymbol{R}|\boldsymbol{\tau}(\boldsymbol{R})\}$ appears unchanged as a coset representative of $\mathcal{T}^{\mathcal{D}}$ in $\mathcal{D}$, then the number or letter corresponding to $\{\boldsymbol{R}|\boldsymbol{\tau}(\boldsymbol{R})\}$ in the symbol for $\mathcal{F}$ is unchanged (Opechowski & Litvin, 1977). The resulting symbol is a symbol for $\mathcal{D}$ based on the symbol for $\mathcal{F}$ and is also a symbol for the magnetic group $\mathcal{M}_R = \mathcal{F}(\mathcal{D})$: the symbol specifies not only $\mathcal{D}$ but also $\mathcal{F}$; by deleting the subindex on the translational part of the symbol and the primes on the rotational part, one obtains the symbol specifying $\mathcal{F}$. Having specified $\mathcal{D}$ and $\mathcal{F}$, one has specified the group $\mathcal{M}_R = \mathcal{F}(\mathcal{D})$.

*Example*

Consider again the group 29.1.198, $\mathcal{F} = Pca2_1$, where

$$\mathcal{F} = \{1|0\}\mathcal{T} \cup \{m_{100}|\tfrac{1}{2}, 0, \tfrac{1}{2}\}\mathcal{T} \cup \{m_{010}|\tfrac{1}{2}, 0, 0\}\mathcal{T} \cup \{2_{001}|0, 0, \tfrac{1}{2}\}\mathcal{T}.$$

The symbol for the $\mathcal{M}_R = \mathcal{F}(\mathcal{D})$ group type 29.7.204 is $P_{2b}c'a'2_1$ and is based on the symbol for $\mathcal{F} = Pca2_1$. The translational subgroup $\mathcal{T}^{\mathcal{D}}$ of $\mathcal{D}$ is given by the symbol $P_{2b}$ where $t_\alpha = \{1|0, 1, 0\}$, *i.e.* $\mathcal{T}^{\mathcal{D}}$ is generated by the three translations $\{1|1, 0, 0\}$, $\{1|0, 2, 0\}$ and $\{1|0, 0, 1\}$ of $\mathcal{T}$, and the translational subgroup $\mathcal{T}^{\mathcal{M}_R}$ of $P_{2b}c'a'2_1$ is given by $\mathcal{T}^{\mathcal{M}_R} = \mathcal{T}^{\mathcal{D}} \cup t_\alpha{}'\mathcal{T}^{\mathcal{D}}$. The two primed symbols $c'$ and $a'$ in $P_{2b}c'a'2_1$ refer to the fact that the two coset representatives $\{m_{100}|\tfrac{1}{2}, 0, \tfrac{1}{2}\}$ and $\{m_{010}|\tfrac{1}{2}, 0, 0\}$ that appear in the set of standard coset representatives of $\mathcal{T}$ in $\mathcal{F}$ appear as the coset representatives $\{m_{100}|\tfrac{1}{2}, 1, \tfrac{1}{2}\}$ and $\{m_{010}|\tfrac{1}{2}, 1, 0\}$ in the set of standard coset representatives of $\mathcal{T}^{\mathcal{D}}$ in $\mathcal{D}$. As the symbol $2_1$ in $P_{2b}c'a'2_1$ is not primed, the coset representative $\{2_{001}|0, 0, \tfrac{1}{2}\}$ of $\mathcal{T}$ in $\mathcal{F}$ remains unchanged as a coset representative of $\mathcal{T}^{\mathcal{D}}$ in $\mathcal{D}$. We have then the subgroup

$$\mathcal{D} = \{1|0\}\mathcal{T}^{\mathcal{D}} \cup \{m_{100}|\tfrac{1}{2}, 1, \tfrac{1}{2}\}\mathcal{T}^{\mathcal{D}} \cup \{m_{010}|\tfrac{1}{2}, 1, 0\}\mathcal{T}^{\mathcal{D}} \cup \{2_{001}|0, 0, \tfrac{1}{2}\}\mathcal{T}^{\mathcal{D}}.$$

We note that these same coset representatives of $\mathcal{T}^{\mathcal{D}}$ in $\mathcal{D}$ are also the coset representatives of the standard set of coset representatives of $\mathcal{T}^{\mathcal{M}_R}$ in $\mathcal{M}_R$.

$$\mathcal{M}_R = \{1|0\}\mathcal{T}^{\mathcal{M}_R} \cup \{m_{100}|\tfrac{1}{2}, 1, \tfrac{1}{2}\}\mathcal{T}^{\mathcal{M}_R} \cup \{m_{010}|\tfrac{1}{2}, 1, 0\}\mathcal{T}^{\mathcal{M}_R} \cup \{2_{001}|0, 0, \tfrac{1}{2}\}\mathcal{T}^{\mathcal{M}_R}$$

and the standard set of coset representatives of $P_{2b}c'a'2_1$ listed in the tables is the same set of coset representatives:

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

Since $\mathcal{T}^{\mathcal{M}_R} = \mathcal{T}^{\mathcal{D}} \cup t_\alpha{}'\mathcal{T}^{\mathcal{D}}$, it follows that $\mathcal{M}_R = \mathcal{D} \cup (\mathcal{F} - \mathcal{D})1'$ and

$$\begin{aligned}\mathcal{M}_R = {}& \{1|0\}\mathcal{T}^{\mathcal{D}} \cup \{m_{100}|\tfrac{1}{2}, 1, \tfrac{1}{2}\}\mathcal{T}^{\mathcal{D}} \cup \{m_{010}|\tfrac{1}{2}, 1, 0\}\mathcal{T}^{\mathcal{D}} \\ & \cup \{2_{001}|0, 0, \tfrac{1}{2}\}\mathcal{T}^{\mathcal{D}} \cup \{1|0, 1, 0\}'\mathcal{T}^{\mathcal{D}} \cup \{m_{100}|\tfrac{1}{2}, 0, \tfrac{1}{2}\}'\mathcal{T}^{\mathcal{D}} \\ & \cup \{m_{010}|\tfrac{1}{2}, 0, 0\}'\mathcal{T}^{\mathcal{D}} \cup \{2_{001}|0, 1, \tfrac{1}{2}\}'\mathcal{T}^{\mathcal{D}}.\end{aligned}$$

Consequently, a primed number or letter in the symbol for $\mathcal{M}_R$ (which is also a symbol for $\mathcal{D}$) denotes that the corresponding coset representative appears in $\mathcal{D}$ coupled with $t_\alpha$ and primed in $(\mathcal{F} - \mathcal{D})1'$, *e.g.* $a'$ in $P_{2b}c'a'2_1$ denotes that the coset $\{m_{100}|\tfrac{1}{2}, 0, \tfrac{1}{2}\}$ appears as $\{m_{100}|\tfrac{1}{2}, 1, \tfrac{1}{2}\}$ in $\mathcal{D}$ and as $\{m_{100}|\tfrac{1}{2}, 0, \tfrac{1}{2}\}'$ in $(\mathcal{F} - \mathcal{D})1'$. An unprimed number or letter in the symbol for $\mathcal{M}_R$ (which is also a symbol for $\mathcal{D}$) denotes that the corresponding element appears unchanged in $\mathcal{D}$ and coupled with $t_\alpha$ and primed in $(\mathcal{F} - \mathcal{D})1'$, *e.g.* the symbol $2_1$ in $P_{2b}c'a'2_1$ denotes that $\{2_{001}|0, 0, \tfrac{1}{2}\}$ is in $\mathcal{D}$ and $\{2_{001}|1, 0, \tfrac{1}{2}\}'$ is in $(\mathcal{F} - \mathcal{D})1'$.

For two-dimensional magnetic space groups with square and hexagonal lattices, three-dimensional magnetic space groups with tetragonal, hexagonal, rhombohedral and cubic lattices, and magnetic layer and rod groups with tetragonal, trigonal or hexagonal lattices, each letter or number in the group type symbol may represent not a single symmetry direction but a set of symmetry directions, see Table 1.3 in Litvin (2013), Table 2.1.3.1 in the present volume and Table 1.2.4.1 in *IT* E. Stokes & Campbell (2009) have pointed out that this can lead to not being able to determine the standard set of coset representatives in $\mathcal{M}_R$ groups from the Opechowski–Guccione magnetic group symbol. Consequently, we introduce the convention that in determining the standard set of coset representatives, each letter or number in the group type symbol in these groups refers to the first symmetry direction of each set of symmetry directions listed in the aforementioned tables.

*Example*

The standard set of coset representatives of 94.1.786 $P4_22_12$ is

$$\begin{array}{llll}\{1|0\}; & \{4_{001}|\tfrac{1}{2}, \tfrac{1}{2}, \tfrac{1}{2}\}; & \{2_{001}|0\}; & \{4_{001}|\tfrac{1}{2}, \tfrac{1}{2}, \tfrac{1}{2}\} \\ \{2_{100}|\tfrac{1}{2}, \tfrac{1}{2}, \tfrac{1}{2}\}; & \{2_{010}|\tfrac{1}{2}, \tfrac{1}{2}, \tfrac{1}{2}\}; & \{2_{110}|0\}; & \{2_{1\bar{1}0}|0\}.\end{array}$$

For the three-dimensional magnetic group 94.7.792 $P_{2c}4_2'2_1'2$, the standard set of coset representatives is

$$\begin{array}{llll}\{1|0\}; & \{4_{001}|\tfrac{1}{2}, \tfrac{1}{2}, \tfrac{3}{2}\}; & \{2_{001}|0, 0, 1\}; & \{4_{001}|\tfrac{1}{2}, \tfrac{1}{2}, \tfrac{1}{2}\} \\ \{2_{100}|\tfrac{1}{2}, \tfrac{1}{2}, \tfrac{3}{2}\}; & \{2_{010}|\tfrac{1}{2}, \tfrac{1}{2}, \tfrac{1}{2}\}; & \{2_{110}|0, 0, 1\}; & \{2_{1\bar{1}0}|0\}.\end{array}$$

The secondary position in the Hermann–Mauguin symbol $P_{2c}4_2'2_1'2$ denotes the set of symmetry directions {[100], [010]}. With this convention, the primed symbol $2_1'$ denotes that the corresponding coset representative $\{2_{100}|\tfrac{1}{2}, \tfrac{1}{2}, \tfrac{1}{2}\}$ of $P4_22_12$ appears in the coset representatives of $P_{2c}4_2'2_1'2$ coupled with the translation $t_\alpha = \{1|0, 0, 1\}$. The third position in the Hermann–Mauguin symbol $P_{2c}4_2'2_1'2$ denotes the set of symmetry directions {[1$\bar{1}$0], [110]}. The unprimed symbol 2 denotes that the coset representative $\{2_{1\bar{1}0}|0\}$ of $P4_22_12$ appears unchanged in the coset representatives of $P_{2c}4_2'2_1'2$.

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**) | $\{1|0\}$ $\{2_{010}|0\}$<br>$\{1|0\}'$ $\{m_{010}|0\}'$ |

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.