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Table 3.6.4.1
Comparisons of three-dimensional OG and BNS magnetic group type symbols

Serial No.	OG	BNS	$\mathcal{F}(\mathcal{D})$
44.1.324	$Imm2$		
44.2.325	$Imm21'$		
44.3.326	$Im'm2'$		
44.4.327	$Im'm'2$		
44.5.328	I_Pmm2	P_Imm2	$Imm2(Pmm2)$
44.6.329	$I_Pmm'2'$	P_Imm2_1	$Imm2(Pmm2_1)$
44.7.330	$I_Pm'm'2$	P_Inn2	$Imm2(Pnn2)$

projection is given with respect to the unit cell of the magnetic group from which it has been projected.

3.6.4. Comparison of OG and BNS magnetic group type symbols

There are other notations for magnetic group type symbols than the notations of Opechowski & Guccione (1965) and Belov, Neronova & Smirnova (1957): for example for the three-dimensional magnetic group 55.10.450 $P_{2c}b'a'm$ the Shubnikov notation is $Ш^{403}_{58}$ (Koptsik, 1966; Shubnikov & Koptsik, 1974) or Sh^{403}_{58} (Ozerov, 1969*a*,*b*) (see also Zamorzaev, 1976). There are also the variations of the Opechowski & Guccione notation put forward by Grimmer (2009, 2010). We shall limit ourselves here to a detailed comparison of the Opechowski & Guccione and Belov, Neronova & Smirnova notations.

For all group types in the reduced magnetic superfamily of $\mathcal{F}$, the Opechowski & Guccione (1965) magnetic group type symbols (OG symbols) are based on the symbol of the group $\mathcal{F}$. Belov, Neronova & Smirnova (1957) also base their symbols (BNS symbols) on the symbol of the group $\mathcal{F}$, but only for magnetic groups of the type $\mathcal{F}$, $\mathcal{F}1'$ and $\mathcal{M}_T$. For magnetic groups $\mathcal{M}_R = \mathcal{F}(\mathcal{D}) = \mathcal{D} \cup (\mathcal{F} - \mathcal{D})1'$, where $\mathcal{D}$ is an equi-class subgroup of $\mathcal{F}$, the BNS symbol is based on the symbol of the group $\mathcal{D}$, the non-primed subgroup of index 2. A magnetic group $\mathcal{M}_R$ can be written as $\mathcal{M}_R = \mathcal{F}(\mathcal{D}) = \mathcal{D} \cup t_\alpha{}'\mathcal{D}$, where t_α is a translation of $\mathcal{F}$ not in $\mathcal{D}$. The BNS symbol for a magnetic group of the type $\mathcal{M}_R$ is the symbol for the group type $\mathcal{D}$ with a subindex inserted on the symbol for the translational subgroup of $\mathcal{D}$ to denote the translation $t_\alpha{}'$.

Example

The representative three-dimensional space group $\mathcal{F} = Pmm2$ has a translational subgroup generated by the three translations $\{1|1, 0, 0\}$, $\{1|0, 1, 0\}$ and $\{1|0, 0, 1\}$ and the standard set of coset representatives

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

The three-dimensional magnetic space group 25.10.165 $\mathcal{F}(\mathcal{D}) = Pmm2(Pcc2)$ has a subgroup $\mathcal{D}$ with a translational subgroup generated by the three translations $\{1|1, 0, 0\}$, $\{1|0, 1, 0\}$ and $\{1|0, 0, 2\}$, $t_\alpha{}' = \{1|0, 0, 1\}'$, and a set of coset representatives

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

The OG magnetic group type symbol is, see Section 3.6.2.2.4, $P_{2c}m'm'2$, *i.e.* based on the symbol for the group type $\mathcal{F} = Pmm2$. The BNS symbol is P_ccc2, *i.e.* based on the symbol for the subgroup $\mathcal{D} = Pcc2$ of $\mathcal{F}$, with a subindex 'c' attached to 'P' to denote the translation $t_\alpha{}' = \{1|0, 0, 1\}'$ in $\mathcal{M}_R = \mathcal{F}(\mathcal{D}) = \mathcal{D} \cup t_\alpha{}'\mathcal{D}$.

A side-by-side comparison of OG magnetic group type symbols and BNS symbols is given in Litvin (2013). As the OG and BNS symbols are the same for magnetic groups $\mathcal{F}$, $\mathcal{F}1'$ and $\mathcal{M}_T$, BNS symbols are explicitly listed only for groups of type $\mathcal{M}_R$. Examples of this comparison are given in Table 3.6.4.1.

3.6.5. Maximal subgroups of index ≤ 4

We consider the maximal subgroups of index ≤ 4 of the one-, two- and three-dimensional magnetic space groups and the two- and three-dimensional magnetic subperiodic groups. A complete listing of the maximal subgroups of the two- and three-dimensional non-primed space groups can be found in *International Tables for Crystallography*, Volume A1, *Symmetry Relations Between Space Groups* (2010; *IT* A1). The maximal subgroups of index ≤ 4 of the three-dimensional non-primed space groups and non-primed layer and rod groups can also be found on the Bilbao Crystallographic Server (http://www.cryst.ehu.es; Aroyo *et al.*, 2006).

For magnetic groups, an abstract of a method for determining the maximal subgroups of magnetic groups was published by Sayari & Billiet (1977). The maximal subgroups of magnetic groups found in Litvin (2013) were derived from Litvin (2008*a*) using a method given by Litvin (1996).

Each maximal subgroup table is headed by the magnetic group type whose maximal subgroup types are to be listed.

Examples

For the three-dimensional magnetic space group type $Pb'a'm$, one finds (Litvin, 2013), in bold blue type, information which defines the representative group of this type in a coordinate system O; **a**, **b**, **c**:

55.5.445 $Pb'a'm$ (0, 0, 0; **a**, **b**, **c**)
$$\begin{array}{ll} \{1|0\} & \{2_{100}|\tfrac{1}{2}, \tfrac{1}{2}, 0\}' \\ \{2_{010}|\tfrac{1}{2}, \tfrac{1}{2}, 0\}' & \{2_{001}|0\} \\ \{\bar{1}|0\} & \{m_{100}|\tfrac{1}{2}, \tfrac{1}{2}, 0\}' \\ \{m_{010}|\tfrac{1}{2}, \tfrac{1}{2}, 0\}' & \{m_{001}|0\} \end{array}$$

The first column gives the global serial number of the group, followed in the second column by its magnetic group type symbol. In the third column, the symbol (O; $\mathbf{a}'$, $\mathbf{b}'$, $\mathbf{c}'$) gives the origin O and basis vectors $\mathbf{a}'$, $\mathbf{b}'$, $\mathbf{c}'$ of the conventional unit cell of the non-primed subgroup of the representative group of the type $Pb'a'm$. These basis vectors $\mathbf{a}'$, $\mathbf{b}'$, $\mathbf{c}'$ imply both the magnetic and non-primed translational subgroups of the representative group. In this case, the P translational subgroup of the representative group is non-primed and generated by the basis vectors **a**, **b**, **c**. The standard set of coset representatives of this representative group is given on the right.

For the three-dimensional magnetic space-group type $P_{2b}ma2$ one finds (Litvin, 2013):

28.6.190 $P_{2b}ma2$ (0, 0, 0; **a**, 2**b**, **c**)
$$\begin{array}{ll} \{1|0\} & \{m_{100}|\tfrac{1}{2}, 0, 0\} \\ \{m_{010}|\tfrac{1}{2}, 0, 0\} & \{2_{001}|0\} \end{array}$$

Note here that $\mathbf{a}' = \mathbf{a}$, $\mathbf{b}' = 2\mathbf{b}$, $\mathbf{c}' = \mathbf{c}$, being the basis vectors of the conventional unit cell of the non-primed subgroup of the representative group of $P_{2b}ma2$, implies that the translational subgroup of the representative group is P_{2b}, *i.e.* generated by the non-primed translations $\{1|1, 0, 0\}$, $\{1|0, 2, 0\}$, $\{1|0, 0, 1\}$ and the magnetic translation $\{1|0, 1, 0\}'$.

Following the subtable heading of each magnetic space-group type is a listing of the maximal subgroups of index ≤ 4 of the representative magnetic space group of this type.

Examples

From the list of maximal subgroups of the representative magnetic group of the type $Pb'a'm$ is the subgroup listed as

$Pb'a'2$	2	$(0, 0, 0; \mathbf{a}, \mathbf{b}, \mathbf{c})$	$\{1\|0\}$	$\{2_{001}\|0\}$
			$\{m_{010}\|\frac{1}{2}, \frac{1}{2}, 0\}'$	$\{m_{100}\|\frac{1}{2}, \frac{1}{2}, 0\}'$

The first column gives the magnetic group type symbol of the subgroup. The second column gives the subgroup index of this subgroup as a subgroup of the representative group of type $Pb'a'm$. In the third column, the symbol $(O + \mathbf{p}; \mathbf{a}', \mathbf{b}', \mathbf{c}')$ gives the origin '$O + \mathbf{p}$' and basis vectors $\mathbf{a}', \mathbf{b}', \mathbf{c}'$ of the conventional unit cell of the non-primed subgroup, where $\mathbf{p}$, a translation of the origin of the coordinate system of the representative group $Pb'a'm$, and the conventional unit cell are such that the coset representatives listed are transformed into the standard cosets of the representative group of the subgroup type $Pb'a'2$. In this case, since the listed coset representatives are the standard cosets of the representative group of type $Pb'a'2$, no translation of origin is required, and consequently $O + \mathbf{p} = 0, 0, 0$. The conventional unit cell of the non-primed subgroup of the subgroup $Pb'a'2$ is the same as that of representative group of the type $Pb'a'2$ and consequently one finds $\mathbf{a}' = \mathbf{a}$, $\mathbf{b}' = \mathbf{b}$, $\mathbf{c}' = \mathbf{c}$.

That the listed coset representatives of the subgroup are the same as those of the representative group of that subgroup type is not always the case:

Example

A subgroup of type $P2/m$ of the representative group $Pb'a'm$ is listed as

$$P2/m \quad 2 \quad (0, 0, 0; \mathbf{b}, \mathbf{c}, \mathbf{a}) \quad \{1|0\}\ \{2_{001}|0\}\ \{\bar{1}|0\}\ \{m_{001}|0\}$$

The standard set of coset representatives of the representative group $P2/m$ are

$$\{1|0\} \quad \{\bar{1}|0\} \quad \{2_{010}|0\} \quad \{m_{010}|0\}.$$

A change in setting to have the coset representatives of the subgroup be identical with the coset representatives of the representative group $P2/m$ is represented in the symbol $(0, 0, 0; \mathbf{b}, \mathbf{c}, \mathbf{a})$, *i.e.* changing the setting from $\mathbf{a}, \mathbf{b}, \mathbf{c}$ to $\mathbf{b}, \mathbf{c}, \mathbf{a}$.

Other cases may require a simultaneous change to both the origin and the setting of the conventional unit cell of the non-primed subgroup:

Example

A third subgroup of the representative group $Pb'a'm$ is the equi-class subgroup of the same type $Pb'a'm$:

$Pb'a'm$	2	$(0, 0, \frac{1}{2}; \mathbf{a}, \mathbf{b}, 2\mathbf{c})$	$\{1\|0\}$	$\{2_{100}\|\frac{1}{2}, \frac{1}{2}, 1\}'$
			$\{2_{010}\|\frac{1}{2}, \frac{1}{2}, 1\}'$	$\{2_{001}\|0\}$
			$\{\bar{1}\|0, 0, 1\}$	$\{m_{100}\|\frac{1}{2}, \frac{1}{2}, 0\}'$
			$\{m_{010}\|\frac{1}{2}, \frac{1}{2}, 0\}'$	$\{m_{001}\|0, 0, 1\}$

The listed coset representatives of this subgroup are not the same as the coset representatives of the representative group $Pb'a'm$, *i.e.* where the z component of the non-primitive translation associated with all coset representatives is zero. To have these listed coset representatives become identical with the coset representatives of the standard representative group of $Pb'a'm$, one must change the origin of the coordinate system. This information is provided in the symbol $(0, 0, \frac{1}{2}; \mathbf{a}, \mathbf{b}, 2\mathbf{c})$ where $O + \mathbf{p} = 0, 0, \frac{1}{2}$ denotes the translation under which all the non-zero z components of the coset representatives are transformed to zero. Note also that the P in the subgroup symbol denotes a non-primed translational subgroup which is determined by $\mathbf{a}' = \mathbf{a}$, $\mathbf{b}' = \mathbf{b}$, $\mathbf{c}' = 2\mathbf{c}$, *i.e.* P denotes the translational group generated by the translations $\{1|1, 0, 0\}$, $\{1|0, 1, 0\}$ and $\{1|0, 0, 2\}$.

In the tabulations of the maximal subgroups of groups of the type $\mathcal{F}1'$ not all maximal subgroups are explicitly listed. The maximal subgroup $\mathcal{F}$ of $\mathcal{F}1'$ is not listed. If $\mathcal{G}$ is a maximal subgroup of $\mathcal{F}$, then $\mathcal{G}1'$ is a maximal subgroup of $\mathcal{F}1'$ and is also not explicitly listed. All maximal subgroups $\mathcal{G}$ of $\mathcal{F}$ are listed under $\mathcal{F}$, and consequently, all maximal subgroups $\mathcal{G}1'$ of $\mathcal{F}1'$ are then found from the list of all maximal subgroups $\mathcal{G}$ of $\mathcal{F}$ by multiplying each by $1'$. For each listed maximal subgroup, its non-primed subgroup type is explicitly given. For example, a listed subgroup of $Pma21'$ is

$Pma'2'$	Pm	2	$(0, 0, 0; \mathbf{a}, \mathbf{b}, \mathbf{c})$	$\{1\|0\}$	$\{2_{001}\|0\}'$
				$\{m_{010}\|\frac{1}{2}, 0, 0\}'$	$\{m_{100}\|\frac{1}{2}, 0, 0\}$

where the non-primed subgroup type Pm of $Pma'2'$ is given in the second column.

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