

3.6. MAGNETIC SUBPERIODIC GROUPS AND MAGNETIC SPACE GROUPS

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	<i>Imm2</i>		
44.2.325	<i>Imm21'</i>		
44.3.326	<i>Im'm2'</i>		
44.4.327	<i>Im'm'2</i>		
44.5.328	<i>I_Pmm2</i>	<i>P₁mm2</i>	<i>Imm2(Pmm2)</i>
44.6.329	<i>I_Pmm'2'</i>	<i>P₁mm2₁</i>	<i>Imm2(Pmm2₁)</i>
44.7.330	<i>I_Pm'm'2</i>	<i>P₁nn2</i>	<i>Imm2(Pnn2)</i>

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 III_{58}^{403} (Koptsik, 1966; Shubnikov & Koptsik, 1974) or Sh_{58}^{403} (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}' 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_α' .

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_{cc}c2*, 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}' 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**:

$$55.5.445 \quad \mathbf{Pb'a'm} \quad (0, 0, 0; \mathbf{a}, \mathbf{b}, \mathbf{c}) \quad \{1|0\} \quad \{2_{100}|\frac{1}{2}, \frac{1}{2}, 0\}' \\ \{2_{010}|\frac{1}{2}, \frac{1}{2}, 0\}' \quad \{2_{001}|0\} \\ \{1|0\} \quad \{m_{100}|\frac{1}{2}, \frac{1}{2}, 0\}' \\ \{m_{010}|\frac{1}{2}, \frac{1}{2}, 0\}' \quad \{m_{001}|0\}$$

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*; **a**', **b**', **c**') gives the origin *O* and basis vectors **a**', **b**', **c**' of the conventional unit cell of the non-primed subgroup of the representative group of the type *Pb'a'm*. These basis vectors **a**', **b**', **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):

$$28.6.190 \quad \mathbf{P}_{2b}ma2 \quad (0, 0, 0; \mathbf{a}, 2\mathbf{b}, \mathbf{c}) \quad \{1|0\} \quad \{m_{100}|\frac{1}{2}, 0, 0\} \\ \{m_{010}|\frac{1}{2}, 0, 0\} \quad \{2_{001}|0\}$$

Note here that **a**' = **a**, **b**' = 2**b**, **c**' = **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.