

3. ADVANCED TOPICS ON SPACE-GROUP SYMMETRY

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, 1935a,b, 1936), i.e. $\{\mathbf{R}|\boldsymbol{\tau}\}$ or $\{\mathbf{R}|\boldsymbol{\tau}'\}$. \mathbf{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 $\{\mathbf{R}|\boldsymbol{\tau}'\}$ is coupled with time inversion. The subindex notation on \mathbf{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}' 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}' 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:

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

ITXC I has been replaced by *IT A*. One 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

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

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 '2₁' in the symbol for $\mathcal{F} = Pca2_1$ refers to the coset representative $\{2_{001}|0, 0, \frac{1}{2}\}$, an element in $\mathcal{D} = P2_1$. Consequently, the symbol '2₁' appears unprimed in the symbol for \mathcal{M}_T ($Pc'a'2_1$) and the coset representative $\{2_{001}|0, 0, \frac{1}{2}\}$ 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 $\{m_{100}|\frac{1}{2}, 0, \frac{1}{2}\}$ and $\{m_{010}|\frac{1}{2}, 0, 0\}$, 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 $\{m_{100}|\frac{1}{2}, 0, \frac{1}{2}\}$ and $\{m_{010}|\frac{1}{2}, 0, 0\}$ 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

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

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