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12.2. Space-group symbols

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12.2.1. Introduction

Each space group is related to a crystallographic point group. Space-group symbols, therefore, can be obtained by a modification of point-group symbols. The simplest modification which merely gives an enumeration of the space-group types (*cf.* Section 8.2.2) has been used by Schoenflies. The Shubnikov and Hermann–Mauguin symbols, however, reveal the glide or screw components of the symmetry operations and are designed in such a way that the nature of the symmetry elements and their relative locations can be deduced from the symbol.

12.2.2. Schoenflies symbols

Space groups related to one point group are distinguished by adding a numerical superscript to the point-group symbol. Thus, the space groups related to the point group C_2 are called C_2^1, C_2^2, C_2^3.

12.2.3. The role of translation parts in the Shubnikov and Hermann–Mauguin symbols

A crystallographic symmetry operation **W** (*cf.* Part 11) is described by a pair of matrices

$$(\boldsymbol{W}, \boldsymbol{w}) = (\boldsymbol{I}, \boldsymbol{w})(\boldsymbol{W}, \boldsymbol{o}).$$

$\boldsymbol{W}$ is called the *rotation part*, $\boldsymbol{w}$ describes the *translation part* and determines the translation vector $\mathbf{w}$ of the operation. $\boldsymbol{w}$ can be decomposed into a *glide/screw part* $\boldsymbol{w}_g$ and a *location part* $\boldsymbol{w}_l : \boldsymbol{w} = \boldsymbol{w}_g + \boldsymbol{w}_l$; here, $\boldsymbol{w}_l$ determines the location of the corresponding symmetry element with respect to the origin. The glide/screw part $\boldsymbol{w}_g$ may be derived by projecting $\boldsymbol{w}$ on the space invariant under $\boldsymbol{W}$, *i.e.* for rotations and reflections $\boldsymbol{w}$ is projected on the corresponding rotation axis or mirror plane. With matrix notation, $\boldsymbol{w}_g$ is determined by $(\boldsymbol{W}, \boldsymbol{w})^k = (\boldsymbol{I}, \boldsymbol{t})$ and $\boldsymbol{w}_g = (1/k)\boldsymbol{t}$, where k is the order of the operation $\boldsymbol{W}$. If $\boldsymbol{w}_g$ is not a symmetry translation, the space group contains sets of screw axes or glide planes instead of the rotation axis or the mirror plane of the related point group. A screw rotation is symbolized by n_m, where $\boldsymbol{w}_g = (m/n)\boldsymbol{t}$, with $\boldsymbol{t}$ the shortest lattice vector in the direction of the rotation axis. The Shubnikov notation and the international notation use the same symbols for screw rotations. The symbols for glide reflections in both notations are listed in Table 12.2.3.1.

If the point-group symbol contains only one generator, the related space group is described completely by the Bravais lattice and a symbol corresponding to that of the point group in which rotations and reflections are replaced by screw rotations or glide reflections, if necessary. If, however, two or more operations generate the point group, it is necessary to have information on the mutual orientations and locations of the corresponding space-group symmetry elements, *i.e.* information on the location components $\boldsymbol{w}$. This is described in the following sections.

12.2.4. Shubnikov symbols

For the description of the mutual orientation of symmetry elements, the same symbols as for point groups are applied. In space groups, however, the symmetry elements need not intersect. In this case, the orientational symbols · (dot), : (colon), / (slash) are modified to $\odot$, $\bigcirc\!\!\!\!:\;$, //. The space-group symbol starts with a description of the lattice defined by the basis **a**, **b**, **c**. For centred cells, the vectors to the centring points are given first. The same letters are used for basis vectors related by symmetry. The relative orientations of the vectors are denoted by the orientational symbols introduced above. The description of the lattice given in parentheses is followed by symbols of the generating elements of the related point group. If necessary, the symbols of the symmetry operations are modified to indicate their glide/screw parts. The first generator is separated from the lattice description by an orientation symbol. If this generator represents a mirror or glide plane, the dot connects the plane with the last two vectors whereas the colon refers only to the last vector. If the generator represents a rotation or a rotoreflection, the colon orients the related axis perpendicular to the plane given by the last two vectors whereas the dot refers only to the last vector. Two generators are separated by the symbols mentioned above to denote their relative orientations and sites. To make this description unique for space groups related to point group $O_h \equiv \tilde{6}/4$ with Bravais lattices cP and cF, it is necessary to use three generators instead of two: $4/\tilde{6} \cdot m$. For the sake of unification, this kind of description is extended to the remaining two space groups having Bravais lattice cI.

Example: *Shubnikov symbol for the space group with Schoenflies symbol* D_{2h}^{26} *(72).*

The Bravais lattice is oI (orthorhombic, body-centred). Therefore, the symbol for the lattice basis is

$$\left(\frac{a+b+c}{2} \Big/ c : (a : b)\right),$$

indicating that there is a centring vector $1/2(\mathbf{a} + \mathbf{b} + \mathbf{c})$ relative to the conventional orthorhombic cell. This vector is oblique with respect to the basis vector **c**, which is orthogonal to the perpendicular pair **a** and **b**. The basis vectors have independent lengths and are thus indicated by different letters a, b and c in arbitrary sequence.

To complete the symbol of the space group, we consider the point group D_{2h}. Its Shubnikov symbol is $m : 2 \cdot m$. Parallel to the (**a**, **b**) plane, there is a glide plane $\widetilde{ab}$ and a mirror plane m. The latter is chosen as generator. From the screw axis 2_1 and the rotation axis 2, both parallel to **c**, the latter is chosen as generator. The third generator can be a glide plane c perpendicular to **b**. Thus the Shubnikov symbol of D_{2h}^{26} is

$$\left(\frac{a+b+c}{2} \Big/ c : (a : b)\right) \cdot m : 2 \cdot \tilde{c}.$$

Table 12.2.3.1. *Symbols of glide planes in the Shubnikov and Hermann–Mauguin space-group symbols*

Glide plane perpendicular to	Glide vector	Shubnikov symbol	Hermann–Mauguin symbol
b or **c**	$\frac{1}{2}\mathbf{a}$	$\tilde{a}$	a
a or **c**	$\frac{1}{2}\mathbf{b}$	$\tilde{b}$	b
a or **b** or **a** − **b**	$\frac{1}{2}\mathbf{c}$	$\tilde{c}$	c
c	$\frac{1}{2}(\mathbf{a}+\mathbf{b})$	$\widetilde{ab}$	n
a	$\frac{1}{2}(\mathbf{b}+\mathbf{c})$	$\widetilde{bc}$	n
b	$\frac{1}{2}(\mathbf{c}+\mathbf{a})$	$\widetilde{ac}$	n
a − **b**	$\frac{1}{2}(\mathbf{a}+\mathbf{b}+\mathbf{c})$	$\widetilde{abc}$	n
c	$\frac{1}{4}(\mathbf{a}+\mathbf{b})$	$\frac{1}{2}\widetilde{ab}$	d
a	$\frac{1}{4}(\mathbf{b}+\mathbf{c})$	$\frac{1}{2}\widetilde{bc}$	d
b	$\frac{1}{4}(\mathbf{c}+\mathbf{a})$	$\frac{1}{2}\widetilde{ac}$	d
a − **b**	$\frac{1}{4}(\mathbf{a}+\mathbf{b}+\mathbf{c})$	$\frac{1}{2}\widetilde{abc}$	d
a + **b**	$\frac{1}{4}(-\mathbf{a}+\mathbf{b}+\mathbf{c})$		d

references