3.3. Space-group symbols and their use

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3.3.1. Point-group symbols

3.3.1.1. Introduction

For symbolizing space groups, or more correctly types of space groups, different notations have been proposed. The following three are the main ones in use today:

(i) the notation of Schoenflies (1891, 1923);

(ii) the notation of Shubnikov (Shubnikov & Koptsik, 1972), which is frequently used in the Russian literature;

(iii) the international notation of Hermann (1928*a*) and Mauguin (1931). This was used in *Internationale Tabellen zur Bestimmung von Kristallstrukturen* (*IT* 1935) and was somewhat modified in *International Tables for X-ray Crystallography* (*IT* 1952).

In all three notations, the space-group symbol is a modification of a point-group symbol.

Symmetry elements occur in lattices, and thus in crystals, only in distinct directions. Point-group symbols make use of these discrete directions and their mutual relations.

3.3.1.2. Schoenflies symbols

Most Schoenflies symbols (Table 3.3.1.3, column 1) consist of the basic parts C_n, D_n,[1] T or O, designating cyclic, dihedral, tetrahedral and octahedral rotation groups, respectively, with $n = 1, 2, 3, 4, 6$. The remaining point groups are described by additional symbols for mirror planes, if present. The subscripts h and v indicate mirror planes perpendicular and parallel to a main axis taken as vertical. For T, the three mutually perpendicular twofold axes and, for O, the three fourfold axes are considered to be the main axes. The index d is used for mirror planes that bisect the angle between two consecutive equivalent rotation axes, *i.e.* which are diagonal with respect to these axes. For the rotoinversion axes $\overline{1}$, $\overline{2} \equiv m$, $\overline{3}$ and $\overline{4}$, which do not fit into the general Schoenflies concept of symbols, other symbols C_i, C_s, C_{3i} and S_4 are in use. The rotoinversion axis $\overline{6}$ is equivalent to $3/m$ and thus designated as C_{3h}.

A detailed introduction to Schoenflies symbols of crystallographic point groups is given in Section 1.4.1.3.

3.3.1.3. Shubnikov symbols

The Shubnikov symbol is constructed from a minimal set of generators of a point group (for exceptions, see below). Thus, strictly speaking, the symbols represent types of symmetry operations. Since each symmetry operation is related to a symmetry element, the symbols also have a geometrical meaning. The Shubnikov symbols for symmetry operations differ slightly from the international symbols (Table 3.3.1.1). Note that Shubnikov, like Schoenflies, regards symmetry operations of the second kind as rotoreflections rather than as rotoinversions.

If more than one generator is required, it is not sufficient to give only the types of the symmetry elements; their mutual orientations must be symbolized too. In the Shubnikov symbol, a dot (·), a colon (:) or a slash (/) is used to designate parallel, perpendicular or oblique arrangement of the symmetry elements. For a reflection, the orientation of the actual mirror plane is considered, not that of its normal. The exception mentioned above is the use of $3 : m$ instead of $\tilde{3}$ in the description of point groups.

[1] Instead of D_2, in older papers V (from *Vierergruppe*) is used.

3.3.1.4. Hermann–Mauguin symbols

3.3.1.4.1. Symmetry directions

The Hermann–Mauguin symbols for finite point groups make use of the fact that the symmetry elements, *i.e.* proper and improper rotation axes, have definite mutual orientations. If for each point group the symmetry directions are grouped into classes of symmetry equivalence, at most three classes are obtained. These classes were called *Blickrichtungssysteme* (Heesch, 1929). If a class contains more than one direction, one of them is chosen as representative.

The Hermann–Mauguin symbols for the crystallographic point groups refer to the symmetry directions of the lattice point groups (holohedries, *cf.* Sections 1.3.4.3 and 3.1.1.4) and use other representatives than chosen by Heesch [*IT* (1935), p. 13]. For instance, in the hexagonal case, the primary set of lattice symmetry directions consists of {[001], [00$\overline{1}$]}, representative is [001]; the secondary set of lattice symmetry directions consists of [100], [010], [$\overline{1}\overline{1}$0] and their counter-directions, representative is [100]; the tertiary set of lattice symmetry directions consists of [1$\overline{1}$0], [120], [$\overline{2}\overline{1}$0] and their counter-directions, representative is [1$\overline{1}$0]. The representatives for the sets of lattice symmetry directions for all lattice point groups are listed in Table 3.3.1.2. The directions are related to the conventional crystallographic basis of each lattice point group (*cf.* Section 3.1.1.4).

The relation between the concept of lattice symmetry directions and group theory is evident. The maximal cyclic subgroups of the maximal rotation group contained in a lattice point group can be divided into, at most, three sets of conjugate subgroups. Each of these sets corresponds to one set of lattice symmetry directions.

Table 3.3.1.1
International (Hermann–Mauguin) and Shubnikov symbols for symmetry elements

The first power of a symmetry operation is often designated by the symmetry-element symbol without exponent 1, the other powers of the operation carry the appropriate exponent.

	Symmetry elements	
	of the first kind	of the second kind
Hermann–Mauguin	1 2 3 4 6	$\overline{1}$ m $\overline{3}$ $\overline{4}$ $\overline{6}$
Shubnikov†	1 2 3 4 6	$\tilde{2}$ m $\tilde{6}$ $\tilde{4}$ $\tilde{3}$

† According to a private communication from J. D. H. Donnay, the symbols for elements of the second kind were proposed by M. J. Buerger. Koptsik (1966) used them for the Shubnikov method.