International Tables for Crystallography (2006). Vol. A, Section 4.3.2.1, p. 62.

4.3. Symbols for space groups

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4.3.1. Triclinic system

There are only two triclinic space groups, $P1$ (1) and $P\bar{1}$ (2). $P1$ is quite outstanding because all its subgroups are also $P1$. They are listed in Table 13.2.2.1 for indices up to [7]. $P\bar{1}$ has subgroups $P\bar{1}$, isomorphic, and $P1$, non-isomorphic.

In the triclinic system, a primitive unit cell can always be selected. In some cases, however, it may be advantageous to select a larger cell, with A, B, C, I or F centring.

The two types of reduced bases (reduced cells) are discussed in Section 9.2.2.

4.3.2. Monoclinic system

4.3.2.1. *Historical note and arrangement of the tables*

In *IT* (1935) only the b axis was considered as the unique axis. In *IT* (1952) two choices were given: the c-axis setting was called the 'first setting' and the b-axis setting was designated the 'second setting'.

To avoid the presence of two standard space-group symbols side by side, in the present tables only *one standard short symbol* has been chosen, that conforming to the long-lasting tradition of the b-axis unique (*cf.* Sections 2.2.4 and 2.2.16). However, for reasons of rigour and completeness, in Table 4.3.2.1 the *full* symbols are given not only for the c-axis and the b-axis settings but also for the a-axis setting. Thus, Table 4.3.2.1 has six columns which in pairs refer to these three settings. In the headline, the unique axis of each setting is underlined.

Additional complications arise from the presence of fractional translations due to glide planes in the primitive cell [groups Pc (7), $P2/c$ (13), $P2_1/c$ (14)], due to centred cells [$C2$ (5), Cm (8), $C2/m$ (12)], or due to both [Cc (9), $C2/c$ (15)]. For these groups, three different choices of the two oblique axes are possible which are called 'cell choices' 1, 2 and 3 (see Section 2.2.16). If this is combined with the three choices of the unique axis, $3 \times 3 = 9$ symbols result. If we add the effect of the permutation of the two oblique axes (and simultaneously reversing the sense of the unique axis to keep the system right-handed, as in **abc** and $\mathbf{c\underline{\bar{b}}a}$), we arrive at the $9 \times 2 = 18$ symbols listed in Table 4.3.2.1 for each of the eight space groups mentioned above.

The space-group symbols $P2$ (3), $P2_1$ (4), Pm (6), $P2/m$ (10) and $P2_1/m$ (11) do not depend on the cell choice: in these cases, one line of six space-group symbols is sufficient.

For space groups with centred lattices (A, B, C, I), extended symbols are given; the 'additional symmetry elements' (due to the centring) are printed in the half line below the space-group symbol.

The use of the present tabulation is illustrated by two examples, Pm, which does not depend on the cell choice, and $C2/c$, which does.

Examples

(1) Pm (6)

(i) *Unique axis b*

In the first column, headed by $\mathbf{a\underline{b}c}$, one finds the full symbol $P1m1$. Interchanging the labels of the oblique axes a and c does not change this symbol, which is found again in the second column headed by $\mathbf{c\underline{\bar{b}}a}$.

(ii) *Unique axis c*

In the third column, headed by $\mathbf{ab\underline{c}}$, one finds the symbol $P11m$. Again, this symbol is conserved in the interchange of the oblique axes a and b, as seen in the fourth column headed by $\mathbf{ba\underline{\bar{c}}}$.

The same applies to the setting with unique axis a, columns five and six.

(2) $C2/c$ (15)

The short symbol $C2/c$ is followed by three lines, corresponding to the cell choices 1, 2, 3. Each line contains six full space-group symbols.

(i) *Unique axis b*

The column headed by $\mathbf{a\underline{b}c}$ contains the three symbols $C\,1\,2/c\,1$, $A1\,2/n\,1$ and $I1\,2/a\,1$, equivalent to the short symbol $C2/c$ and corresponding to the cell choices 1, 2, 3. In the half line below each symbol, the additional symmetry elements are indicated (extended symbol). If the oblique axes a and c are interchanged, the column under $\mathbf{c\underline{b}a}$ lists the symbols $A1\,2/a\,1$, $C1\,2/n\,1$ and $I1\,2/c\,1$ for the three cell choices.

(ii) *Unique axis c*

The column under $\mathbf{ab\underline{c}}$ contains the symbols $A112/a$, $B112/n$ and $I112/b$, corresponding to the cell choices 1, 2 and 3. If the oblique axes a and b are interchanged, the column under $\mathbf{ba\underline{\bar{c}}}$ applies.

Similar considerations apply to the a-axis setting.

4.3.2.2. *Transformation of space-group symbols*

How does a monoclinic space-group symbol transform for the various settings of the same unit cell? This can be easily recognized with the help of the headline of Table 4.3.2.1, completed to the following scheme:

$\mathbf{a\underline{b}c}$	$\mathbf{c\underline{\bar{b}}a}$	**cab**	$\mathbf{ac\bar{b}}$	**bca**	$\mathbf{\bar{b}ac}$	Unique axis b
bca	$\mathbf{a\bar{c}b}$	$\mathbf{ab\underline{c}}$	$\mathbf{ba\underline{\bar{c}}}$	**cab**	$\mathbf{\bar{c}ba}$	Unique axis c
cab	$\mathbf{b\bar{a}c}$	**bca**	$\mathbf{cb\bar{a}}$	$\mathbf{\underline{a}bc}$	$\mathbf{\underline{\bar{a}}cb}$	Unique axis a.

The use of this three-line scheme is illustrated by the following examples.

Examples

(1) $C2/c$ (15, unique axis b, cell choice 1)

Extended symbol: $C1\,2/c\,1$.
$2_1/n$

Consider the setting **cab**, first line, third column. Compared to the initial setting $\mathbf{a\underline{b}c}$, it contains the 'unique axis b' in the third place and, consequently, must be identified with the setting $\mathbf{ab\underline{c}}$, unique axis c, in the third column, for which in Table 4.3.2.1 the new symbol for cell choice 1 is listed as $A11\,2/a$
$2_1/n$.

(2) $C2/c$ (15, unique axis b, cell choice 3)

Extended symbol: $I1\,2/a\,\,1$.
$2_1/c$

Consider the setting $\mathbf{\bar{b}ac}$ in the first line, sixth column. It contains the 'unique axis b' in the first place and thus must be identified with the setting $\mathbf{\underline{\bar{a}}cb}$, unique axis a, in the sixth column. From Table 4.3.2.1, the appropriate space-group symbol for cell choice 3 is found as $I\,2/b\,11$.
$2_1/c$

4.3.2.3. *Group–subgroup relations*

It is easy to read all monoclinic maximal t and k subgroups of types **I** and **IIa** directly from the extended full symbols of a space group. Maximal subgroups of types **IIb** and **IIc** cannot be recognized by simple inspection of the synoptic Table 4.3.2.1

references