1, enlargement in any direction;

2, *mm*2, 3, 3*m*, 4, 4*mm*, 6 and 6*mm*, enlargement in the direction of the unique axis;

m, enlargement parallel to the plane of symmetry.

Example 3.1.5.1.2.

The cell enlargement **a**, **b**, 5**c** of space group $Cmc2_1$, No. 36, (crystal class *mm*2) does not produce conjugate subgroups.

If one is unsure whether conjugate subgroups exist, this can be looked up in the tables of Chapter 2.3 of this volume, where all conjugate subgroups are always mentioned and joined by a left brace.

Example 3.1.5.1.3.

For space group $Pm\bar{3}m$, No. 221, two subgroups $Im\bar{3}m$ ($2\mathbf{a}, 2\mathbf{b}, 2\mathbf{c}$) with index 4 are listed. Each of them belongs to a set of four conjugate subgroups which differ in their origin locations $(0,0,0; -1,0,0; 0,-1,0; 0,0,-1$ for the first listed subgroup, referred to the coordinate system of $Pm\bar{3}m$). This can be seen by the coordinate values to be added $(0,0,0; \frac{1}{2},0,0; 0,\frac{1}{2},0; 0,0,\frac{1}{2}$; coordinate system of $Im\bar{3}m$). In Chapter 2.3, all four conjugate subgroups and their origin shifts are listed and joined by a brace.

3.1.5.2. *Orientational conjugation*

In this case, the conjugate subgroups have differently oriented unit cells that are equivalent by a symmetry operation other than a translation of the space group. This occurs in the following cases: orthorhombic subgroups of hexagonal space groups; monoclinic subgroups of trigonal (including rhombohedral) space groups; rhombohedral and tetragonal subgroups of cubic space groups. In these cases, the corresponding cell and coordinate transformations are listed for all conjugate subgroups after the word 'conjugate'. Their Wyckoff symbols, being the same for all conjugate subgroups, are not repeated.

Example 3.1.5.2.1.

The cubic space group $P\bar{4}3m$, No. 215, has three tetragonal conjugate subgroups $P\bar{4}2m$. Their tetragonal *c* axes correspond to the cubic *a*, *b* or *c* axes, respectively. In $P\bar{4}3m$, *a*, *b* and *c* are symmetry-equivalent by the threefold rotation axes.

3.1.6. Monoclinic and triclinic subgroups

Aside from the two choices for the unique axis and the three possible cell choices given in Volume A, the unit cell of a monoclinic space group allows many more settings that can be interconverted by transformations such as $\mathbf{a} \pm q\mathbf{c}, \mathbf{b}, \mathbf{c}$ with an integer value for *q* (Sayari & Billiet, 1977). The most commonly chosen cell is the one with the shortest basis vectors **a** and **c** and a non-acute angle β. For triclinic space groups the 'reduced' cell is preferred, which depends on the metric values of the lattice (Billiet & Rolley Le Coz, 1980).

Some relations always require a cell transformation, for example rhombohedral to monoclinic relations. A group–subgroup relation in which the subgroup is monoclinic or triclinic can always be chosen together with a cell transformation that produces one of the cells mentioned. The transformation to be chosen depends on the cell metrics of the starting space group. For general tables we therefore cannot specify *a priori* the kind of cell transformation that will be needed.

The settings listed for monoclinic and triclinic subgroups were chosen in such a way that axes transformations are avoided or kept to a minimum. Depending on the cell metrics, this may result in cells that do not have the shortest possible basis vectors. Unfortunately, transformation of a monoclinic or triclinic cell setting to another one may cause an interchange of Wyckoff labels (within the Wyckoff sets). Frequently, several possible cell settings of the same monoclinic subgroup have been listed; the entry for the subgroup then is followed by the word 'or' or 'alternative', plus another entry.

Example 3.1.6.1.

Space group *Cmcm*, No. 63, has the subgroup $P112_1/m$, No. 11. It requires a cell transformation which is given as $\mathbf{a}, \frac{1}{2}(-\mathbf{a}+\mathbf{b}), \mathbf{c}$. The following two lines list two other possible cell transformations for the *same* subgroup after the words 'or': $\frac{1}{2}(\mathbf{a}-\mathbf{b}), \mathbf{b}, \mathbf{c}$ and $\frac{1}{2}(\mathbf{a}-\mathbf{b}), \frac{1}{2}(\mathbf{a}+\mathbf{b}), \mathbf{c}$. These three options cause different relations for the Wyckoff positions 4*b* and 8*d* of *Cmcm*.

Caution should also be exerted when different cell choices of monoclinic cells are involved. Monoclinic subgroups may refer to any of the three cell choices listed in Volume A. As long as these cell choices are used as listed in Volume A, no problems should arise. However, interconversions from one setting to another and especially nonconventional settings require special attention.

Example 3.1.6.2.

The common setting of space group No. 15 is $C12/c1$, which means unique axis *b* and cell choice 1; the glide plane *c* is located at $y = 0$ (and $y = \frac{1}{2}$). By interchanging the axes **b** and $-\mathbf{c}$, $C12/c1$ becomes $B112/b$ with the *b* glide plane at $z = 0$. This was the setting listed in *International Tables for X-ray Crystallography* (1952, 1965, 1969) for unique axis *c*. However, since the 1983 edition of Volume A, $B112/b$ does not correspond to one of the listed cell choices. Instead, they are now $A112/a$ (cell choice 1) or $B112/n$ (cell choice 2) or $I112/b$ (cell choice 3). Note that for all three cell choices the glide plane mentioned in the symbol is at $z = 0$. $B112/n$ also has a glide plane in the **b** direction, but unlike $B112/b$ it is at $z = \frac{1}{4}$. $B112/n$ and $B112/b$ can be set up with the same unit-cell dimensions, but with origins shifted by $\frac{1}{4}, 0, \frac{1}{4}$. The full Hermann–Mauguin symbol always shows uniquely which is the setting.