These are HM symbols of space groups in conventional settings. It is less easy to find the conventional HM symbol and the space-group type from an unconventional short HM symbol. This may be seen from the following example:

Question: Given the short HM symbols *Pman*, *Pmbn* and *Pmcn*, what are the conventional descriptions of their space-group types, and are they identical or different?

Answer: A glance at the HM symbols shows that the second symbol does not describe any space-group type at all. The second symmetry direction is **b**; the glide plane is perpendicular to it and the glide component may be $\frac{1}{2}\mathbf{a}$, $\frac{1}{2}\mathbf{c}$ or $\frac{1}{2}(\mathbf{c}+\mathbf{a})$, but not $\frac{1}{2}\mathbf{b}$.

In this case it is convenient to define the intersection of the three (glide) reflection planes as the site of the origin. Then all translation components of the generators are zero except the glide components.

(1) *Pman*. If one names the three (glide) reflections according to the directions of their normals by m_{100}, a_{010} and n_{001}, then $a_{010}n_{001} = 2_{100}$, $m_{100}a_{010} = 2_{001}$, while the composition $n_{001}m_{100}$ results in a 2_1 screw rotation along [010].

Clearly, the unconventional full HM symbol is $P\,2/m\,2_1/a\,2/n$. The procedure for obtaining from this symbol the conventional HM symbol $P\,2/m\,2/n\,2_1/a$ (or short symbol *Pmna*) with the origin at the inversion centre is described in Chapter 1.5.

(2) *Pmcn*. Using a nomenclature similar to that of (1), one obtains 2_1 screw axes along [100], [010] and [001] by the compositons $c_{010}n_{001}$, $n_{001}m_{100}$ and $m_{100}c_{010}$, respectively. Thus the unconventional full HM symbol is $P\,2_1/m\,2_1/c\,2_1/n$. Again, the procedure of Chapter 1.5 results in the full HM symbol $P\,2_1/n\,2_1/m\,2_1/a$ or the short symbol *Pnma*. The full HM symbols show that the two space-group types are different.

1.4.1.4.6. Tetragonal space groups

There are seven tetragonal crystal classes. The lattice may be *P* or *I*. The space groups of the three crystal classes 4, $\overline{4}$ and 4/*m* have only one symmetry direction, [001]. The other four classes, 422, 4*mm*, $\overline{4}2m$ and 4/*m* 2/*m* 2/*m* display three symmetry directions which are listed in the sequence [001], [100] and [1$\overline{1}$0].[5]

1.4.1.4.6.1. Tetragonal space groups with one symmetry direction

In the space groups of the crystal class 4, rotation or screw rotation axes run in direction [001]; in the space groups of crystal class $\overline{4}$ these are rotoinversion axes $\overline{4}$; and in crystal class 4/*m* both occur. The rotation 4 of the point group may be replaced by screw rotations 4_1, 4_2 or 4_3 in the space groups with a *P* lattice. If the lattice is *I*-centred, 4 and 4_2 or 4_1 and 4_3 occur simultaneously, together with $\overline{4}$ rotoinversions.

In the space groups of crystal class 4/*m* with a *P* lattice, the rotations 4 can be replaced by the screw rotations 4_2 and the reflection *m* by the glide reflection *n* such that four space-group types with a *P* lattice exist: *P*4/*m*, $P4_2/m$, *P*4/*n* and $P4_2/n$. Two more are based on an *I* lattice: *I*4/*m* and $I4_1/a$. In all these six space groups the short HM symbols and full HM symbols are the same.

[5] One usually chooses [1$\overline{1}$0] as the representative direction and not the equivalent direction [110], in analogy to the cases of trigonal and hexagonal space groups where [1$\overline{1}$0] is the representative of the set of tertiary symmetry directions, while [$\overline{1}\overline{1}$0] (or [110]) belongs to the set of secondary symmetry directions, *cf.* Table 2.1.3.1.

1.4.1.4.6.2. Tetragonal space groups with three symmetry directions

There are four crystal classes with three symmetry directions each. In the corresponding space-group symbols the constituents 2, 4 and *m* may be replaced by 2_1, 4_k with *k* = 1, 2 or 3, and *a*, *b*, *c*, *n* or *d*, respectively. The constituent $\overline{4}$ persists. Full HM symbols of space groups are, among others, $P4_22_12$, $P4_2bc$, $P\overline{4}2c$ and $I\,4_1/a\,2/c\,2/d$.

The full and short HM symbols agree for the space groups that belong to the crystal classes 422, 4*mm* and $\overline{4}2m$. Only for the space groups of 4/*m* 2/*m* 2/*m* have the short HM symbols lost their twofold rotations or screw rotations leading, *e.g.*, to the symbol $I4_1/acd$ instead of $I\,4_1/a\,2/c\,2/d$.

Example

In *P*4*mm*, to the primary symmetry direction [001] belong the rotation 4 and its powers, to the secondary symmetry direction [100] belongs the reflection m_{100}. However, in the tertiary symmetry direction [1$\overline{1}$0], there occur reflections *m* and glide reflections *g* with a glide vector $\frac{1}{2}(\mathbf{a}+\mathbf{b})$. Such glide reflections are not listed in the 'symmetry operations' blocks of the space-group tables if they are composed of a representing *general position* and an integer translation, as happens here (*cf.* Section 1.4.2.4 and Section 1.5.4 for a detailed discussion of the additional symmetry operations generated by combinations with integer translations). Glide reflections may have complicated glide vectors. If these do not fit the labels *a*, *b*, *c*, *n* or *d*, they are frequently called *g*.

1.4.1.4.7. Trigonal, hexagonal and rhombohedral space groups

Hexagonal and trigonal space groups are referred to a hexagonal coordinate system *P* with basis vector $\mathbf{c} \perp (\mathbf{a}, \mathbf{b})$. The basis vectors **a** and **b** span a hexagonal net and form an angle of 120°. The sequence of the representatives of the (up to three) symmetry directions is [001], [100] and [1$\overline{1}$0]. Usually, the seven trigonal space groups of the rhombohedral lattice system (or *rhombohedral space groups* for short) are described either with respect to a hexagonal coordinate system (triple hexagonal cell) or to a rhombohedral coordinate system (primitive rhombohedral cell).

1.4.1.4.7.1. Trigonal space groups

Trigonal space groups are characterized by threefold rotation or screw rotation or rotoinversion axes in [001]. There may be in addition 2 and 2_1 axes in [100] or [1$\overline{1}$0], but only in one of these two directions. The same holds for reflections *m* or glide reflections *c*. The different possibilities are:

(1) There are only threefold axes 3 or 3_1 or 3_2 or $\overline{3}$. The short and the full HM symbols are *P*3, $P3_1$, $P3_2$, $P\overline{3}$.

(2) There are in addition horizontal twofold axes. Their direction is either [100] or [1$\overline{1}$0]. The corresponding position of the HM symbol is marked by 2, the other (empty) position is marked by 1: *P*321, *P*312, $P3_121$, $P3_112$ *etc. Note*: *P*321 and *P*312 denote *different* space-group types.

(3) In addition to the threefold axes, there are reflection planes or glide planes with their representative normals in the horizontal directions [100] or [1$\overline{1}$0]. The corresponding position of the HM symbol is marked by *m* or *c*, the empty position is marked by 1: *P*3*m*1 or *P*31*m etc.*

(4) The main axis in [001] is $\overline{3}$. Because $\overline{3}$ contains an inversion, the second or third position in the full HM symbol is marked by 2/*m* or 2/*c*, which leads to the HM symbols $P\,\overline{3}\,2/m\,1$ or