$P\bar{1}$ is the only one which displays the inversion $\bar{1}$ explicitly. Sometimes non-conventional centred lattice descriptions may be used, especially when comparing crystal structures.

1.4.1.4.4. Monoclinic space groups

Monoclinic space groups have exactly one symmetry direction, often called *the monoclinic axis*. The *b* axis is the symmetry direction of the (most frequently used) conventional setting, called the *b*-axis setting. Another conventional setting has **c** as its symmetry direction (*c*-axis setting). In earlier literature, the unique-axis *c* setting was called the first setting and the unique-axis *b* setting the second setting (*cf.* Section 2.1.3.15). In addition to the primitive lattice *P* there is a centred lattice which is taken as *C* in the *b*-axis setting, *A* in the *c*-axis setting. The (possible) glide reflections are *c* (or *a*). In this volume, more settings are described, *cf.* Sections 1.5.4 and 2.1.3.15 and the space-group tables of Chapter 2.3.

The full HM symbol consists of the lattice symbol and three possible positions for the symmetry directions. The symmetry in the **a** direction is described first, followed by the symmetry in the **b** direction and last in the **c** direction. The two positions of the HM symbol that are not occupied by the monoclinic symmetry direction are marked by 1. The symbol is thus similar to the orthorhombic HM symbol and the monoclinic axis is clearly visible. *P*1*m*1 or *P*11*m* may designate the same space group but in different settings. *Pm*11 is a possible but not conventional setting.

The short HM symbols of the monoclinic space groups are independent of the setting of the space group. They form the *monoclinic standard symbols* and are not variable: *P*2, $P2_1$, *C*2, *Pm*, *Pc*, *Cm*, *Cc*, *P*2/*m*, $P2_1/m$, *C*2/*m*, *P*2/*c*, $P2_1/c$ and *C*2/*c*. Altogether there are 13 monoclinic space-group types.

There are several reasons for the many conventional settings.

(1) As only one of the three coordinate axes is fixed by symmetry, there are two conventions related to the possible permutations of the other axes.

(2) The sequence of the three coordinate axes may be chosen because of the lengths of the basis vectors, *i.e.* not because of symmetry.

(3) If two different crystal structures have related symmetries, one being a subgroup of the other, then it is often convenient to choose a non-conventional setting for one of the structures to make their structural relations transparent. Such similarity happens in particular in substances that are related by a non-destructive phase transition. Monoclinic space groups are particularly flexible in their settings.

1.4.1.4.5. Orthorhombic space groups

To the orthorhombic crystal system belong the crystal classes 222, *mm*2 and 2/*m* 2/*m* 2/*m* with the Bravais types of lattices *P*, *C*, *A*, *F* and *I*. Four space groups with a *P* lattice belong to the crystal class 222, ten to *mm*2 and 16 to 2/*m* 2/*m* 2/*m*. Each of the basis vectors marks a symmetry direction; the lattice symbol is followed by characters representing the symmetry operations with respect to the symmetry directions along **a**, **b** and **c**.

We start with the full HM symbols. For a space group of crystal class 222 with a *P* lattice the HM symbol is thus '$PR_1R_2R_3$', where $R_1, R_2, R_3 = 2$ or 2_1. Conventionally one chooses a setting with the symbols *P*222, $P222_1$, $P2_12_12$ and $P2_12_12_1$.

For the generation of the space groups of this crystal class only two non-translational generators are necessary, say R_1 and R_2. However, it is not possible to indicate in the HM symbol whether the axes R_1 and R_2 intersect or not. This is decided by the third (screw) rotation R_3: if $R_3 = R_1R_2 = 2$, the axes R_1 and R_2 intersect, if $R_3 = 2_1$, they do not. For this reason, R_3 is sometimes called an *indicator*. However, any two of the three rotations or screw rotations can be taken as the generators and the third one is then the indicator. Mathematically each element of a generating set is a generator independent of its possible redundancy.

In the space groups of crystal class *mm*2 the two reflections or glide reflections are the generators, the twofold rotation or screw rotation is generated by composition of the (glide) reflections. The position of the rotation axis relative to the intersection line of the two planes as well as its screw component are determined uniquely by the glide components of the reflections or glide reflections.

The rotation or screw rotation in the HM symbols of space groups of the crystal class *mm*2 could be omitted, and were omitted in older HM symbols. Nowadays they are included to make the orthorhombic HM symbols more homogeneous. Conventional symbols are, among others, *Pmm*2, $Pmc2_1$, *Pba*2 and $Pca2_1$.

The 16 space groups with a *P* lattice in crystal class 2/*m* 2/*m* 2/*m* are similarly obtained by starting with the letter *P* and continuing with the point-group symbol, modified by the possible replacements 2_1 for 2 and *a*, *b*, *c* or *n* for *m*. The conventional symbols are, among others, $P2/m\,2/m\,2/m$, $P2_1/m\,2/m\,2/a$, $P2/m\,2/n\,2_1/a$, $P2_1/b\,2_1/a\,2/m$ or $P2_1/n\,2_1/m\,2_1/a$. The symbols $P2/m\,2/n\,2_1/a$ and $P2_1/n\,2_1/m\,2_1/a$ designate different space-group types, as is easily seen by looking at the screw rotations: $P2/m\,2/n\,2_1/a$ has screw axes in the direction of **c** only, $P2_1/n\,2_1/m\,2_1/a$ has screw axes in all three symmetry directions.

If the lattice is centred, the constituents in the same symmetry direction are not unique. In this case, according to the 'simplest symmetry operation' rule, in general the simplest operation is chosen, *cf.* Section 1.5.4.

Examples

In the HM symbol $C2/m\,2/c\,2_1/m$ there are in addition 2_1 screw rotations in the first two symmetry directions; additional glide reflections *b* occur in the first, and *n* in the second and third symmetry directions.

In *I*2/*b* 2/*a* 2/*m*, all rotations 2 are accompanied by screw rotations 2_1; *b* and *a* are accompanied by *c* and *m* is accompanied by *n*. The symmetry operations that are not listed in the full HM symbol can be derived by composition of the listed operations with a centring translation, *cf.* Section 1.4.2.4.

There are two exceptions to the 'simplest symmetry operation' rule. If the *I* centring is added to the *P* space groups of the crystal class 222, one obtains two different space groups with an *I* lattice, each has 2 and 2_1 operations in each of the symmetry directions. One space group is derived by adding the *I* centring to the space group *P*222, the other is obtained by adding the *I* centring to a space group $P2_12_12_1$. In the first case the twofold axes intersect, in the second they do not. According to the rules both should get the HM symbol *I*222, but only the space group generated from *P*222 is named *I*222, whereas the space group generated from $P2_12_12_1$ is called $I2_12_12_1$. The second exception occurs among the cubic space groups and is due to similar reasons, *cf.* Section 1.4.1.4.8.

The *short HM symbols* for the space groups of the crystal classes 222 and *mm*2 are the same as the full HM symbols. In the short HM symbols for the space groups of the crystal class 2/*m* 2/*m* 2/*m* the symbols for the (screw) rotations are omitted, resulting in the short symbols *Pmmm*, *Pmma*, *Pmna*, *Pbam*, *Pnma*, *Cmcm* and *Ibam* for the space groups mentioned above.

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