of a screw component. Therefore, reflections and glide reflections can better express the geometric relations between the symmetry operations than can rotations and screw rotations; reflections and glide reflections are more important for HM symbols than are rotations and screw rotations. The latter are frequently omitted to form short HM symbols from the full ones.

The second part of the *full HM symbol* of a space group consists of one position for each of up to three representative symmetry directions. To each position belong the generating symmetry operations of their representative symmetry direction. The position is thus occupied either by a rotation, screw rotation or rotoinversion and/or by a reflection or glide reflection.

The representative symmetry directions are different in the different crystal systems. For example, the directions of the basis vectors **a**, **b** and **c** are symmetry independent in orthorhombic crystals and are thus all representative, whereas **a** and **b** are symmetry equivalent and thus dependent in tetragonal crystals. All three directions are symmetry equivalent in cubic crystals; they belong to the same set and are represented by one of the directions. Therefore, the symmetry directions and their sequence in the HM symbols depend on the crystal system to which the crystal and thus its space group belongs.

Table 1.4.1.1 gives the positions of the representative lattice-symmetry directions in the HM symbols for the different crystal systems.

Examples of full HM symbols are (from triclinic to cubic) $P\bar{1}$, $P12/c1$, $A112/m$, $F2/d\,2/d\,2/d$, $I4_1/a$, $P4/m\,2_1/n\,2/c$, $P\bar{3}$, $P3m1$, $P3_112$, $R\bar{3}2/c$, $P6_3/m$, $P6_122$ and $F4_132$.

There are crystal systems, for example tetragonal, for which the high-symmetry space groups display symmetry in all symmetry directions whereas lower-symmetry space groups display symmetry in only some of them. In such cases, the symmetry of the 'empty' symmetry direction is denoted by the constituent 1 or it is simply omitted. For example, instead of three symmetry directions in $P4mm$, there is only one in $I4_1/a11$, for which the HM symbol is usually written $I4_1/a$. However, in some trigonal space groups the designation of a symmetry direction by '1' ($P3_112$) is necessary to maintain the uniqueness of the HM symbols.[4]

The HM symbols can not only describe the space groups in their conventional settings but they can also indicate the setting of the space group relative to the conventional coordinate system mentioned in Section 1.4.1.3.1. For example, the orthorhombic space group $P2/m\,2/n\,2_1/a$ may appear as $P2/n\,2/m\,2_1/b$ or $P2/n\,2_1/c\,2/m$ or $P2_1/c\,2/n\,2/m$ or $P2_1/b\,2/m\,2/n$ or $P2/m\,2_1/a\,2/n$ depending on its orientation relative to the conventional coordinate basis. On the one hand this is an advantage, because the HM symbols include some indication of the orientation of the space group and form a more powerful tool than being just a space-group nomenclature. On the other hand, it is sometimes not easy to recognize the space-group type that is described by an unconventional HM symbol. In Section 1.4.1.4.5 an example is provided which deals with this problem.

[4] In the original HM symbols the constituent '1' was avoided by the use of different centred cells.

Table 1.4.1.1
The structure of the Hermann–Mauguin symbols for the space groups

The positions of the representative symmetry directions for the different crystal systems are given. The description of the non-translational part of the HM symbol is always preceded by the lattice symbol, which in conventional settings is *P*, *A*, *B*, *C*, *F*, *I* or *R*. For monoclinic **b** setting and monoclinic **c** setting, *cf.* Section 1.4.1.4.4; the primitive hexagonal lattice is called *H* in this table.

Crystal system	First position	Second position	Third position
Triclinic (anorthic)	1 or $\bar{1}$	—	—
Monoclinic **b** setting Monoclinic **c** setting	1 1	**b** 1	1 **c**
Orthorhombic	**a**	**b**	**c**
Tetragonal	**c**	**a**	**a** − **b**
Trigonal *H* lattice	**c** **c**	**a** or 1	1 **a** − **b**
Trigonal, *R* lattice, hexagonal coordinates Trigonal, *R* lattice, rhombohedral coordinates	$\mathbf{c}_H$ $\mathbf{a}_R + \mathbf{b}_R + \mathbf{c}_R$	$\mathbf{a}_H$ or $\mathbf{a}_R - \mathbf{b}_R$	— —
Hexagonal	**c**	**a**	**a** − **b**
Cubic	**c**	**a** + **b** + **c**	**a** − **b**

The full HM symbols describe the symmetry of a space group in a transparent way, but they are redundant. They can be shortened to the *short HM symbols* such that the set of generators is reduced to a necessary set. Examples will be displayed for the different crystal systems. The *conventional short HM symbols* still provide a unique description and enable the generation of the space group. For the monoclinic space groups with their many conventional settings they are not variable and are taken as standard for their space-group types. Monoclinic short HM symbols may look quite different from the full HM symbol, *e.g.* Cc instead of $A1n1$ or $I1a1$ or $B11n$ or $I11b$.

The *extended HM symbols* display the additional symmetry that is often generated by lattice centrings. The full HM symbol denotes only the simplest symmetry operations for each symmetry direction, by the 'simplest symmetry operation' rule; the other operations can be found in the extended symbols, which are treated in detail in Section 1.5.4 and are listed in Tables 1.5.4.3 (plane groups) and 1.5.4.4 (space groups).

From the HM symbol of the space group, the full or short *HM symbol for a crystal class* of a space group is obtained easily: one omits the lattice symbol, cancels all screw components such that only the symbol for the rotation is left and replaces any letter for a glide reflection by the letter *m* for a reflection. Examples are $P2_1/b\,2_1/a\,2/m \rightarrow 2/m\,2/m\,2/m$ and $I4_1/a11 \rightarrow 4/m$.

If one is not yet familiar with the HM symbols, it is recommended to start with the orthorhombic space groups in Section 1.4.1.4.5. In the orthorhombic crystal system all crystal classes have the same number of symmetry directions and the HM symbols are particularly transparent. Therefore, the orthorhombic HM symbols are explained in more detail than those of the other crystal systems.

The following discussion treats mainly the HM symbols of space groups in conventional settings; for non-conventional descriptions of space groups the reader is referred to Chapter 1.5.

1.4.1.4.3. Triclinic space groups

There is no symmetry direction in a triclinic space group. Therefore, the basis vectors of a triclinic space group can always be chosen to span a primitive cell and the HM symbols are $P1$ (without inversions) and $P\bar{1}$ (with inversions). The HM symbol

$P\bar{1}$ 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, *P*2/*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 $I2/b\,2/a\,2/m$, 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.