

## 1.4. SPACE GROUPS AND THEIR DESCRIPTIONS

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)  $P\bar{1}$ ,  $P12/c1$ ,  $A112/m$ ,  $F2/d2/d2/d$ ,  $I4_1/a$ ,  $P4/m2_1/n2/c$ ,  $P\bar{3}$ ,  $P3m1$ ,  $P3_112$ ,  $R\bar{3}2/c$ ,  $P6_3/m$ ,  $P6_322$  and  $F4_32$ .

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.<sup>4</sup>

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  $P2/m2/n2_1/a$  may appear as  $P2/n2/m2_1/b$  or  $P2/n2_1/c2/m$  or  $P2_1/c2/n2/m$  or  $P2_1/b2/m2/n$  or  $P2/m2_1/a2/n$  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.

**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>b</b> setting Monoclinic <b>c</b> setting	1 1	<b>b</b> 1	1 <b>c</b>
Orthorhombic	<b>a</b>	<b>b</b>	<b>c</b>
Tetragonal	<b>c</b>	<b>a</b>	<b>a – b</b>
Trigonal <i>H</i> lattice	<b>c</b> <b>c</b>	<b>a</b> or 1	1 <b>a – b</b>
Trigonal, <i>R</i> lattice, hexagonal coordinates	<b>c<sub>H</sub></b>	<b>a<sub>H</sub></b> or <b>a<sub>R</sub> – b<sub>R</sub></b>	—
Trigonal, <i>R</i> lattice, rhombohedral coordinates	<b>a<sub>R</sub> + b<sub>R</sub> + c<sub>R</sub></b>	<b>a<sub>R</sub> – b<sub>R</sub></b>	—
Hexagonal	<b>c</b>	<b>a</b>	<b>a – b</b>
Cubic	<b>c</b>	<b>a + b + c</b>	<b>a – b</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 centring. 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  $P2_1/b2_1/a2/m \rightarrow 2/m2/m2/m$  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

<sup>4</sup> In the original HM symbols the constituent '1' was avoided by the use of different centred cells.