

1.4. SPACE GROUPS AND THEIR DESCRIPTIONS

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 \mathbf{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 $P2/m2_1/a2/n$. The procedure for obtaining from this symbol the conventional HM symbol $P2/m2/n2_1/a$ (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 compositions $c_{010}n_{001}$, $n_{001}m_{100}$ and $m_{100}c_{010}$, respectively. Thus the unconventional full HM symbol is $P2_1/m2_1/c2_1/n$. Again, the procedure of Chapter 1.5 results in the full HM symbol $P2_1/n2_1/m2_1/a$ 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 , $\bar{4}$ and $4/m$ have only one symmetry direction, $[001]$. The other four classes, 422 , $4mm$, $\bar{4}2m$ and $4/m2/m2/m$ display three symmetry directions which are listed in the sequence $[001]$, $[100]$ and $[1\bar{1}0]$.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 $\bar{4}$ these are rotoinversion axes $\bar{4}$; 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 $\bar{4}$ 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: $P4/m$, $P4_2/m$, $P4/n$ and $P4_2/n$. Two more are based on an I lattice: $I4/m$ 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 $[1\bar{1}0]$ as the representative direction and not the equivalent direction $[110]$, in analogy to the cases of trigonal and hexagonal space groups where $[1\bar{1}0]$ is the representative of the set of tertiary symmetry directions, while $[\bar{1}\bar{1}0]$ (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 $\bar{4}$ persists. Full HM symbols of space groups are, among others, $P4_22_12$, $P4_2bc$, $P\bar{4}2c$ and $I4_1/a2/c2/d$.

The full and short HM symbols agree for the space groups that belong to the crystal classes 422 , $4mm$ and $\bar{4}2m$. Only for the space groups of $4/m2/m2/m$ have the short HM symbols lost their twofold rotations or screw rotations leading, e.g., to the symbol $I4_1/acd$ instead of $I4_1/a2/c2/d$.

Example

In $P4mm$, 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 $[1\bar{1}0]$, 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 \mathbf{a} and \mathbf{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 $[1\bar{1}0]$. 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 $[1\bar{1}0]$, 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 $\bar{3}$. The short and the full HM symbols are $P3$, $P3_1$, $P3_2$, $P\bar{3}$.
- (2) There are in addition horizontal twofold axes. Their direction is either $[100]$ or $[1\bar{1}0]$. The corresponding position of the HM symbol is marked by 2 , the other (empty) position is marked by 1 : $P321$, $P312$, $P3_121$, $P3_112$ etc. Note: $P321$ and $P312$ 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 $[1\bar{1}0]$. The corresponding position of the HM symbol is marked by m or c , the empty position is marked by 1 : $P3m1$ or $P31m$ etc.
- (4) The main axis in $[001]$ is $\bar{3}$. Because $\bar{3}$ 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 $P\bar{3}2/m1$ or

1. INTRODUCTION TO SPACE-GROUP SYMMETRY

$P\bar{3}12/m$ etc. In the short HM symbol the ‘2’ is not kept: $P\bar{3}m1$ or $P\bar{3}1m$ etc.

1.4.1.4.7.2. Hexagonal space groups

Hexagonal space groups have either one or three representative symmetry directions. The space groups of crystal classes 6 , $\bar{6}$ and $6/m$ have $[001]$ as their single symmetry direction for the axis 6 or 6_k for $k = 1, \dots, 5$ or $\bar{6}$, and for the plane m with its normal along $[001]$. The short and full HM symbols are the same. Examples are $P6$, $P6_4$, $P\bar{6}$ and $P6_3/m$.

Space groups of crystal classes 622 , $6mm$, $\bar{6}2m$ and $6/m\ 2/m\ 2/m$ have the representative symmetry directions $[001]$, $[100]$ and $[\bar{1}\bar{1}0]$. As opposed to the trigonal HM symbols, in the hexagonal HM symbols no symmetry direction is ‘empty’ and occupied by ‘1’.

In space groups of the crystal classes 622 , $6mm$ and $\bar{6}2m$ the short and full HM symbols are the same; in $6/m\ 2/m\ 2/m$ the short symbols are deprived of the parts ‘2’ of the full symbols. The full HM symbol $P6_3/m\ 2/m\ 2/c$ is shortened to the short HM symbol $P6_3/mmc$, the full HM symbol $P6_3/m\ 2/c\ 2/m$ is shortened to $P6_3/mcm$. The two denote different space-group types.

1.4.1.4.7.3. Rhombohedral space groups

The rhombohedral lattice may be understood as an R -centred hexagonal lattice and then referred to the hexagonal basis. It has two kinds of symmetry directions, which coincide with the primary and secondary symmetry directions of the hexagonal lattice (owing to the R centring, no symmetry operation along the tertiary symmetry direction of the hexagonal lattice is compatible with the rhombohedral lattice). On the other hand, the rhombohedral lattice may be referred to a (primitive) rhombohedral coordinate system with the lattice parameters $a = b = c$ and $\alpha = \beta = \gamma$. The HM symbol of a rhombohedral space group starts with R , its representative symmetry directions are $[001]_{\text{hex}}$ or $[111]_{\text{rhom}}$ and $[100]_{\text{hex}}$ or $[\bar{1}\bar{1}0]_{\text{rhom}}$. In this section the rhombohedral primitive cell is used. The rotations 3 and the rotoinversions $\bar{3}$ are accompanied by screw rotations 3_1 and 3_2 . Rotations 2 about horizontal axes always alternate with 2_1 screw rotations and reflections m are accompanied by different glide reflections g with unconventional glide components. The additional operations mentioned are not listed in the full HM symbols.

The seven rhombohedral space groups belong to the five crystal classes 3 , $\bar{3}$, 32 , $3m$ and $\bar{3}2/m$. In $R3$ and $R\bar{3}$ only the first of the symmetry directions is occupied and listed in the full and short HM symbols. In the space groups of the other crystal classes the second symmetry direction $[\bar{1}\bar{1}0]$ is occupied by ‘2’ or ‘ m ’ or ‘ c ’ or ‘ $2m$ ’ or ‘ $2c$ ’, leading to the full HM symbols $R32$, $R3m$, $R3c$, $R\bar{3}2/m$ and $R\bar{3}2/c$. In the short HM symbols the ‘2’ parts of the last two symbols are skipped: $R\bar{3}m$ and $R\bar{3}c$.

1.4.1.4.8. Cubic space groups

There are five cubic crystal classes combined with the three types of lattices P , F and I in which the cubic space groups are classified. The two symmetry directions $[100]$ and $[111]$ are the representative directions in the space groups of the crystal classes 23 and $2/m\bar{3}$. A third representative symmetry direction, $[\bar{1}\bar{1}0]$, is added for space groups of the crystal classes 432 , $\bar{4}3m$ and $4/m\bar{3}2/m$.⁶

⁶ Note: ‘3’ or ‘ $\bar{3}$ ’ directly after the lattice symbol denotes a trigonal or rhombohedral space group; ‘3’ or ‘ $\bar{3}$ ’ in the third position (second position after the lattice symbol) is characteristic for cubic space groups.

Table 1.4.1.2

The structure of the Hermann–Mauguin symbols for the plane groups

The positions of the representative symmetry directions for the crystal systems are given. The lattice symbol and the maximal order of rotations around a point are followed by two positions for symmetry directions.

Crystal system	Lattice(s)	First position	Second position	Third position
Oblique	p	1 or 2	—	—
Rectangular	p, c	1 or 2	a	b
Tetragonal	p	4	a	a – b
Hexagonal	p	3	a or 1	1 a – b
		3	1	a – b
		6	a	a – b

In the full HM symbol the symmetry is described as usual. Examples are $P2_13$, $F2/d\bar{3}$, $P4_332$, $F\bar{4}3c$, $P4_2/m\bar{3}2/n$ and finally No. 230, $I4_1/a\bar{3}2/d$. The short HM symbols of the noncentrosymmetric space groups (those of crystal classes 23 , 432 and $\bar{4}3m$) are the same as the full HM symbols. In the short HM symbols of centrosymmetric space groups of the crystal classes $2/m\bar{3}$ and $4/m\bar{3}2/m$ the rotations or screw rotations are omitted with the exception of the rotations 3 and rotoinversions $\bar{3}$ which represent the symmetry in direction $[111]$. Thus, in the examples listed above, $Fd\bar{3}$, $Pm\bar{3}n$ and $Ia\bar{3}d$ are the short HM symbols differing from the full HM symbols.

As in the orthorhombic space groups $I222$ and $I2_12_12_1$, there is the pair $I23$ and $I2_13$ in which the ‘simplest symmetry operation’ rule is violated. In both space groups twofold rotations and screw rotations around **a**, **b** and **c** occur simultaneously. In $I23$ the rotation axes intersect, in $I2_13$ they do not. The first space group can be generated by adding the I -centring to the space group $P23$, the second is obtained by adding the I -centring to the space group $P2_13$.

1.4.1.5. Hermann–Mauguin symbols of the plane groups

The principles of the HM symbols for space groups are retained in the HM symbols for plane groups (also known as *wallpaper groups*). The rotation axes along **c** of three dimensions are replaced by *rotation points* in the **ab** plane; the possible orders of rotations are the same as in three-dimensional space: 2, 3, 4 and 6. The lattice (sometimes called *net*) of a plane group is spanned by the two basis vectors **a** and **b**, and is designated by a lower-case letter. The choice of a lattice basis, *i.e.* of a minimal cell, leads to a primitive lattice p , in addition a c -centred lattice is conventionally used. The nets are listed in Table 3.1.2.1. The reflections and glide reflections through planes of the space groups are replaced by *reflections and glide reflections through lines*. Glide reflections are called g independent of the direction of the glide line. The arrangement of the constituents in the HM symbol is displayed in Table 1.4.1.2.

Short HM symbols are used only if there is at most one symmetry direction, *e.g.* $p411$ is replaced by $p4$ (no symmetry direction), $p1m1$ is replaced by pm (one symmetry direction) *etc.*

There are four crystal systems of plane groups, *cf.* Table 3.2.3.1. The analogue of the triclinic crystal system is called *oblique*, the analogues of the monoclinic and orthorhombic crystal systems are *rectangular*. Both have rotations of order 2 at most. The presence of reflection or glide reflection lines in the rectangular crystal system allows one to choose a rectangular basis with one basis vector perpendicular to a symmetry line and one basis