

## 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  $4/m\bar{3}2/m$ .<sup>6</sup>

<sup>6</sup> 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	<b>a</b>	<b>b</b>
Tetragonal	$p$	4	<b>a</b>	<b>a – b</b>
Hexagonal	$p$	3	<b>a</b> or 1	1
		3	1	<b>a – b</b>
		6	<b>a</b>	<b>a – b</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

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vector parallel to it. The *square* crystal system is analogous to the tetragonal crystal system for space groups by the occurrence of fourfold rotation points and a square net. Plane groups with threefold and sixfold rotation points are united in the *hexagonal* crystal system with a hexagonal net.

Plane groups occur as sections and projections of the space groups, *cf.* Section 1.4.5. In order to maintain the relations to the space groups, the symmetry directions of the symmetry lines are determined by their normals, not by the directions of the lines themselves. This is important because the normal of the line, not the direction of the line itself, determines the position in the HM symbol.

- (1) In oblique plane groups there is no symmetry direction: HM symbols are  $p1$  or  $p2$ .
- (2) Rectangular plane groups may have no rotations and then only one symmetry direction:  $p1m1 = pm$ ,  $p1g1 = pg$  and  $c1m1 = cm$ . If there are twofold rotations, the HM symbol starts with  $p2$  or  $c2$ , followed by the symmetry  $m$  or  $g$  first perpendicular to  $\mathbf{a}$  and then perpendicular to  $\mathbf{b}$ . The conventional HM symbol  $p2mg$  describes a plane group with a reflection line running perpendicular to  $\mathbf{a}$  (parallel to  $\mathbf{b}$ ) and a glide-reflection line running from the back to the front (perpendicular to  $\mathbf{b}$  and thus parallel to  $\mathbf{a}$ ). There are four plane-group types:  $p2mm$ ,  $p2mg$ ,  $p2gg$  and  $c2mm$ . The constituent '2' was sometimes omitted in older HM symbols.
- (3) There is one square plane group with only rotations and no symmetry directions, the net is a square net:  $p411 = p4$ . The generating symmetry of symmetry directions perpendicular to  $\mathbf{a}$  and  $\mathbf{a} - \mathbf{b}$  are listed in the second and third positions:  $p4mm$  with reflection lines perpendicular to  $\mathbf{a}$  and  $\mathbf{b}$  and  $p4gm$  with glide lines in the same directions. Reflection lines and glide lines perpendicular to  $\mathbf{a} - \mathbf{b}$  (and  $\mathbf{a} + \mathbf{b}$ ) alternate.
- (4) Five plane groups belong to the hexagonal crystal system. The trigonal and hexagonal plane groups  $p311 = p3$  and  $p611 = p6$  contain only rotations. In the other trigonal plane groups there is exactly one set of symmetry directions; its representative direction is either perpendicular to  $\mathbf{a}$  ( $p3m1$ ) or perpendicular to  $\mathbf{a} - \mathbf{b}$  ( $p31m$ ).

The HM symbols  $p3m1$  and  $p31m$  may be easily confused, although they are different. Apart from the different orientations of their symmetry directions, in a plane group of type  $p3m1$ , all rotation points lie on reflection lines, but in  $p31m$  not all of them do.

The hexagonal plane group  $p6mm$  displays representative directions of mirror lines perpendicular to  $\mathbf{a}$  and perpendicular to  $\mathbf{a} - \mathbf{b}$ .

### 1.4.1.6. Sequence of space-group types

The sequence of space-group entries in the space-group tables follows that introduced by Schoenflies (1891) and is thus established historically. Within each geometric crystal class, Schoenflies numbered the space-group types in an obscure way. As early as 1919, Niggli (1919) considered this Schoenflies sequence to be unsatisfactory and suggested that another sequence might be more appropriate. Fedorov (1891) used a different sequence in order to distinguish between symmorphic, hemisymorphic and asymmorphic space groups (*cf.* Section 1.3.3.3 for a detailed discussion of symmorphic space groups).

The basis of the Schoenflies symbols and thus of the Schoenflies listing is the geometric crystal class. For the present space-group tables, a sequence might have been preferred in which, in addition, space-group types belonging to the same arithmetic

**Table 1.4.1.3**

List of geometric crystal classes in which the Schoenflies sequence separates space groups belonging to the same arithmetic crystal class

Geometric crystal class	Space-group type		
	No.	Hermann–Mauguin symbol	Schoenflies symbol
$2/m$	10	$P2/m$	$C_{2h}^1$
	11	$P2_1/m$	$C_{2h}^2$
	13	$P2/c$	$C_{2h}^4$
	14	$P2_1/c$	$C_{2h}^5$
	12	$C2/m$	$C_{2h}^3$
	15	$C2/c$	$C_{2h}^6$
32	149	$P312$	$D_3^1$
	151	$P3_112$	$D_3^2$
	153	$P3_212$	$D_3^3$
	150	$P321$	$D_3^4$
	152	$P3_121$	$D_3^5$
	154	$P3_221$	$D_3^6$
$3m$	156	$P3m1$	$C_{3v}^1$
	158	$P3c1$	$C_{3v}^3$
	157	$P31m$	$C_{3v}^2$
	159	$P31c$	$C_{3v}^4$
	160	$R3m$	$C_{3v}^5$
	161	$R3c$	$C_{3v}^6$
23	195	$P23$	$T^1$
	198	$P2_13$	$T^4$
	196	$F23$	$T^2$
	197	$I23$	$T^3$
	199	$I2_13$	$T^5$
$m\bar{3}$	200	$Pm\bar{3}$	$T_h^1$
	201	$Pn\bar{3}$	$T_h^2$
	205	$Pa\bar{3}$	$T_h^6$
	202	$Fm\bar{3}$	$T_h^3$
	203	$Fd\bar{3}$	$T_h^4$
	204	$Im\bar{3}$	$T_h^5$
432	206	$Ia\bar{3}$	$T_h^7$
	207	$P432$	$O^1$
	208	$P4_232$	$O^2$
	213	$P4_132$	$O^7$
	212	$P4_332$	$O^6$
	209	$F432$	$O^3$
	210	$F4_132$	$O^4$
	211	$I432$	$O^5$
214	$I4_132$	$O^8$	
$\bar{4}3m$	215	$P\bar{4}3m$	$T_d^1$
	218	$P\bar{4}3n$	$T_d^4$
	216	$F\bar{4}3m$	$T_d^2$
	219	$F\bar{4}3c$	$T_d^5$
	217	$I\bar{4}3m$	$T_d^3$
	220	$I\bar{4}3d$	$T_d^6$

crystal class were grouped together. It was decided, however, that the long-established sequence in the earlier editions of *International Tables* should not be changed.

In Table 1.4.1.3, those geometric crystal classes are listed in which the Schoenflies sequence separates space groups belonging to the same arithmetic crystal class (*cf.* Section 1.3.4.4 for the definition and discussion of arithmetic crystal classes). The space