

1.4. SPACE GROUPS AND THEIR DESCRIPTIONS

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
23	195	$P23$	T^1
	198	$P2_13$	T^4
	196	$F23$	T^2
	197	$I23$	T^3
$m\bar{3}$	199	$I2_13$	T^5
	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
$\bar{4}3m$	214	$I4_132$	O^8
	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