

## 1. INTRODUCTION TO SPACE-GROUP SYMMETRY

primitive lattice. In  $Fmm2$  (42) for example, three additional lines appear in the extended symbol, namely  $ba2$ ,  $nc2_1$  and  $cn2_1$ . These operations are obtained by combining successively the centring translations  $t(\frac{1}{2}, \frac{1}{2}, 0)$ ,  $t(0, \frac{1}{2}, \frac{1}{2})$  and  $t(\frac{1}{2}, 0, \frac{1}{2})$  with the symmetry operations of  $Pmm2$ . However, in space groups  $Fdd2$  (43) and  $Fddd$  (70) the nature of the  $d$  planes is not altered by the translations of the  $F$ -centred lattice; for this reason, in Table 1.5.4.4 a two-line symbol for  $Fdd2$  and a one-line symbol for  $Fddd$  are sufficient.

In tetragonal space groups with primitive lattices there are no alternating symmetry operations belonging to the symmetry directions  $[001]$  and  $[100]$ . However, for the symmetry direction  $[1\bar{1}0]$  the symmetry operations  $2$  and  $2_1$  alternate, as do the reflection  $m$  and the glide reflection  $g$  [ $g$  is the name for a glide reflection with a glide vector  $(\frac{1}{2}, \frac{1}{2}, 0)$ ], and the glide reflections  $c$  and  $n$ . For example, the second line of the extended symbol of  $P4_2/n2/b2/c$  (133) contains the expression  $2_1/n$  under the expression  $2/c$ .

For the space groups in the tetragonal system, the unique axis is always the  $c$  axis, thus reducing the number of settings and choices of the unit cell. Two additional multiple cells are considered in this system, namely the  $C$  and  $F$  cells obtained from the  $P$  and  $I$  cell by the following relations:

$$\mathbf{a}' = \mathbf{a} \mp \mathbf{b}; \quad \mathbf{b}' = \pm \mathbf{a} + \mathbf{b}; \quad \mathbf{c}' = \mathbf{c}.$$

The secondary  $[100]$  and tertiary  $[110]$  symmetry directions are interchanged in this cell transformation. As an example, consider  $P4/n$  (85) and its description with respect to a  $C$ -centred basis. Under the transformation  $\mathbf{a}' = \mathbf{a} + \mathbf{b}$ ,  $\mathbf{b}' = -\mathbf{a} + \mathbf{b}$ ,  $\mathbf{c}' = \mathbf{c}$ , the  $n$  glide  $n(\frac{1}{2}, \frac{1}{2}, 0)$   $x, y, 0$  is transformed to an  $a$  glide  $a$   $x, y, 0$  while its coplanar equivalent glide  $n(-\frac{1}{2}, \frac{1}{2}, 0)$   $x, y, 0$  is transformed to a  $b$  glide  $b$   $x, y, 0$ . Thus, the extended symbol of the multiple-cell description of  $P4/n$  (85) shown in Table 1.5.4.4 is  $C4/a(b)$ , while in accordance with the  $e$ -glide convention, the short Hermann–Mauguin symbol becomes  $C4/e$ .

In the case of  $I4/m$  (87), as a result of the  $I$  centring, screw rotations  $4_2$  and glide reflections  $n$  normal to  $4_2$  appear as additional symmetry operations and are shown in the second line of the extended symbol (cf. Table 1.5.4.4). In the multiple-cell setting, the space group  $F4/m$  exhibits the additional fourfold screw axis  $4_2$  and owing to the new orientation of the  $a'$  and  $b'$  axes, which are rotated by  $45^\circ$  relative to the original axes  $a$  and  $b$ , the  $n$  glide of  $I4/m$  becomes an  $a$  glide in the extended Hermann–Mauguin symbol. The additional  $b$  glide obtained from a coplanar  $n$  glide is not given explicitly in the extended symbol.

The rhombohedral space groups are listed together with the trigonal space groups under the heading ‘Trigonal system’. For both representative symmetry directions  $[001]_{\text{hex}}$  and  $[100]_{\text{hex}}$ , rotations with screw rotations and reflections with glide reflections or different kinds of glide reflections alternate, so that additional symmetry operations always occur: rotations  $3$  or rotoinversions  $\bar{3}$  are accompanied by  $3_1$  and  $3_2$  screw rotations;  $2$  rotations alternate with  $2_1$  screw rotations and  $m$  reflections or  $c$  glide reflections alternate with additional glide reflections. As examples, under the full Hermann–Mauguin symbol  $R3$  (146) one finds  $3_{1,2}$  and in the line under  $R\bar{3}2/c$  (167) one finds  $3_{1,2}$   $2_1/n$ .

The extended Hermann–Mauguin symbols for space groups of the hexagonal crystal system retain the symbol for the primary symmetry direction  $[001]$ . Along the secondary  $(100)$  and tertiary  $(1\bar{1}0)$  symmetry directions every horizontal axis  $2$  is accompanied by a screw rotation  $2_1$ , while the reflections and glide reflections, or different types of glide reflections, alternate.

The list of hexagonal and trigonal space-group symbols is completed by a multiple  $H$  cell, which is three times the volume of the corresponding  $P$  cell. The unit-cell transformation is obtained from the relation

$$\mathbf{a}' = \mathbf{a} - \mathbf{b}; \quad \mathbf{b}' = \mathbf{a} + 2\mathbf{b}; \quad \mathbf{c}' = \mathbf{c}$$

with centring points at  $0, 0, 0$ ;  $\frac{2}{3}, \frac{1}{3}, 0$  and  $\frac{1}{3}, \frac{2}{3}, 0$ . The new vectors  $\mathbf{a}'$  and  $\mathbf{b}'$  are rotated by  $-30^\circ$  in the  $ab$  plane with respect to the old vectors  $\mathbf{a}$  and  $\mathbf{b}$ . There are altogether six possible such multiple cells rotated by  $\pm 30^\circ$ ,  $\pm 90^\circ$  and  $\pm 150^\circ$  (cf. Table 1.5.1.1 and Fig. 1.5.1.8).

The hexagonal lattice is frequently referred to the orthorhombic  $C$ -centred cell (cf. Table 1.5.1.1 and Fig. 1.5.1.7). The volume of this centred cell is twice the volume of the primitive hexagonal cell and its basis vectors are mutually perpendicular.

In general, the space groups of the cubic system do not yield any additional orientations and only the short, full and extended symbols are given. The only exception to this general rule is the group  $Pa\bar{3}$  (205) with its alternative setting  $Pb\bar{3}$ , whose basis vectors  $\mathbf{a}'$ ,  $\mathbf{b}'$ ,  $\mathbf{c}'$  are related by a rotation of  $90^\circ$  in the  $ab$  plane to the basis vectors  $\mathbf{a}$ ,  $\mathbf{b}$ ,  $\mathbf{c}$  of  $Pa\bar{3}$ :  $\mathbf{a}' = \mathbf{b}$ ,  $\mathbf{b}' = -\mathbf{a}$ ,  $\mathbf{c}' = \mathbf{c}$ . The different general reflection conditions of  $Pb\bar{3}$  in comparison to those of  $Pa\bar{3}$  indicate its importance for diffraction studies (cf. Table 1.6.4.25). In some extended symbols of the cubic groups, we note the use of the  $g$  or  $g_i$  type of glide reflections as in, for example,  $F\bar{4}3c$  (219). The  $g$  glide is a generic form of a glide plane which is different from the usual glide planes denoted by  $a$ ,  $b$ ,  $c$ ,  $n$ ,  $d$  or  $e$ . The symbols  $g$ ,  $g_1$  and  $g_2$  indicate specific glide components and orientations that are specified in the *Note* to Table 1.5.4.4.

## References

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