

## 1. INTRODUCTION TO SPACE-GROUP SYMMETRY

Table 1.5.4.3

List of plane-group symbols

System and lattice symbol	Point group	No. of plane group	Hermann–Mauguin symbol			Full symbol for other setting	Multiple cell
			Short	Full	Extended		
Oblique <i>p</i>	1	1		<i>p</i> 1			
	2	2		<i>p</i> 2			
Rectangular <i>p, c</i>	<i>m</i>	{ 3 4 5	<i>pm</i>	<i>p</i> 1 <i>m</i> 1	<i>c</i> 1 <i>m</i> 1 <i>g</i>	<i>p</i> 11 <i>m</i>	
			<i>pg</i>	<i>p</i> 1 <i>g</i> 1		<i>p</i> 11 <i>g</i>	
<i>cm</i>			<i>c</i> 1 <i>m</i> 1	<i>c</i> 11 <i>m</i>			
	<i>2mm</i>	{ 6 7 8 9		<i>p</i> 2 <i>mm</i>	<i>c</i> 2 <i>mm</i> <i>g g</i>	<i>p</i> 2 <i>mm</i>	
			<i>p</i> 2 <i>m</i> g	<i>p</i> 2 <i>gm</i>			
			<i>p</i> 2 <i>g</i> g	<i>p</i> 2 <i>gg</i>			
			<i>c</i> 2 <i>mm</i>	<i>c</i> 2 <i>mm</i>			
Square <i>p</i>	4	10		<i>p</i> 4	<i>p</i> 4 <i>mm</i> <i>g</i> <i>p</i> 4 <i>gm</i> <i>g</i>		<i>c</i> 4 <i>c</i> 4 <i>mm</i> <i>g</i> <i>c</i> 4 <i>mg</i> <i>g</i>
	<i>4mm</i>	{ 11		<i>p</i> 4 <i>mm</i>			
		12		<i>p</i> 4 <i>gm</i>			
Hexagonal <i>p</i>	3	13		<i>p</i> 3	<i>p</i> 3 <i>m</i> 1 <i>g</i> <i>p</i> 31 <i>m</i> <i>g</i> <i>p</i> 6 <i>p</i> 6 <i>mm</i> <i>g g</i>		<i>h</i> 3 <i>h</i> 31 <i>m</i> <i>g</i> <i>h</i> 3 <i>m</i> 1 <i>g</i> <i>h</i> 6 <i>h</i> 6 <i>mm</i> <i>g g</i>
	<i>3m</i>	{ 14		<i>p</i> 3 <i>m</i> 1			
		15		<i>p</i> 31 <i>m</i>			
		16		<i>p</i> 6			
	<i>6mm</i>	17		<i>p</i> 6 <i>mm</i>			

rotations 2 and screw rotations  $2_1$  and  $c$  and  $n$  glide reflections alternate, and thus under the full symbol  $C12/c1$  one finds the entry  $2_1/n$ .

In Table 1.5.4.4 the Hermann–Mauguin symbols of the orthorhombic space groups are listed in six different settings: the *standard setting abc*, and the settings *ba $\bar{c}$* , *cab*,  *$\bar{c}ba$* , *bca* and *a $\bar{c}b$* . These six settings result from the possible permutations of the three axes. Let us compare for a few space groups the standard setting *abc* with the *cab* setting. For  $Pmm2$  (25) the permutation yields the new setting  $P2mm$ , reflecting the fact that the twofold axes parallel to the  $c$  direction change to the  $a$  direction. The mirrors normal to  $a$  and  $b$  become normal to  $b$  and  $c$ , respectively.

The case of  $Cmm2$  (35) is slightly more complex due to the centring. As a result of the permutation the  $C$  centring becomes an  $A$  centring. The changes in the twofold axes and mirrors are similar to those of the previous example and result in the  $A2mm$  setting of  $Cmm2$ .

The extended Hermann–Mauguin symbol of the centred space group  $Aem2$  (39) reveals the nature of the  $e$ -glide plane (also called the ‘double’ glide plane): among the set of glide reflections through the same (100) plane, there exist two glide reflections with glide components  $\frac{1}{2}b$  and  $\frac{1}{2}c$  (for details of the  $e$ -glide notation the reader is referred to Section 1.2.3, see also de Wolff *et al.*, 1992). In the *cab* setting, the  $A$  centring changes to a  $B$  centring and the double glide plane is now normal to  $b$  and the glide reflections have glide components  $\frac{1}{2}a$  and  $\frac{1}{2}c$ . The corresponding symbol is thus  $B2em$ . Note that in the cases of the five orthorhombic space groups whose Hermann–Mauguin symbols contain the  $e$ -glide symbol, namely  $Aem2$  (39),  $Aea2$  (41),  $Cmce$  (64),  $Cmme$  (67) and  $Ccce$  (68), the characters in the first lines of the extended symbols differ from the short symbols because the characters in the extended symbol represent symmetry operations, whereas those in the short and full symbol represent symmetry elements. In all these cases, the extended symbols

listed in Table 1.5.4.4 are complemented by the short symbols, given in brackets.

The general discussion in Section 1.5.4.1 about the additional symmetry operations that occur as a result of combinations with lattice translations provides some rules for the construction of the extended Hermann–Mauguin symbols in the orthorhombic crystal system. In orthorhombic space groups with primitive lattices, the symmetry operations of any symmetry direction are always unique: either 2 or  $2_1$ , either  $m$  or  $a$  or  $b$  or  $c$  or  $n$ . In  $C$ -centred lattices, owing to the possible combination of the original symmetry operations with the centring translations, the axes 2 along [100] and [010] alternate with axes  $2_1$ . However, parallel to  $c$  there are either 2 or  $2_1$  axes because the combination of a rotation or screw rotation with a centring translation results in another operation of the same kind. Similarly,  $m_{100}$  alternates with  $b_{100}$ ,  $m_{010}$  with  $a_{010}$ ,  $c_{100}$  with  $n_{100}$  etc. The  $m_{001}$  reflection plane is simultaneously an  $n_{001}$  glide plane and an  $a_{001}$  glide plane is simultaneously a  $b_{001}$  glide plane. This latter plane with its double role is the  $e_{001}$  glide plane, as found for example in the full symbol of  $C2/m2/m2/e$  (67) and the corresponding short symbol  $Cmme$ . As another example, consider the space group  $C2/m2/c2_1/m$  (63). In Table 1.5.4.4, in the line of various settings for this space group the short Hermann–Mauguin symbols are listed, and the rotations or screw rotations do not appear. The  $m_{100}$ ,  $c_{010}$  and  $m_{001}$  reflections and glide reflections occur alternating with  $b_{100}$ ,  $n_{010}$  and  $n_{001}$  glide reflections, respectively. The entry under  $Cmcm$  is thus  $bnn$ .

$F$  and  $I$  centring cause alternating symmetry operations for all three coordinate axes  $a$ ,  $b$  and  $c$ . For these centring, the permutation of the axes does not affect the symbol  $F$  or  $I$  of the centring type. However, the number of symmetry operations increases by a factor of four for  $F$  centring and by a factor of two for  $I$  centring when compared to those of a space group with a

(continued on page 106)