2. GUIDE TO THE USE OF THE SPACE-GROUP TABLES

(iii) *Relations between the basis vectors* $\mathbf{a}'$, $\mathbf{b}'$ *of the plane group and the basis vectors* $\mathbf{a}$, $\mathbf{b}$, $\mathbf{c}$ *of the space group.* Each set of basis vectors refers to the conventional coordinate system of the plane group or space group, as employed in Parts 6 and 7. The basis vectors of the two-dimensional cell are always called $\mathbf{a}'$ and $\mathbf{b}'$ irrespective of which two of the basis vectors $\mathbf{a}$, $\mathbf{b}$, $\mathbf{c}$ of the three-dimensional cell are projected to form the plane cell. All relations between the basis vectors of the two cells are expressed as vector equations, *i.e.* $\mathbf{a}'$ and $\mathbf{b}'$ are given as linear combinations of $\mathbf{a}$, $\mathbf{b}$ and $\mathbf{c}$. For the triclinic or monoclinic space groups, basis vectors $\mathbf{a}$, $\mathbf{b}$ or $\mathbf{c}$ inclined to the plane of projection are replaced by the projected vectors $\mathbf{a}_p, \mathbf{b}_p, \mathbf{c}_p$.

For primitive three-dimensional cells, the *metrical* relations between the lattice parameters of the space group and the plane group are collected in Table 2.2.14.1. The additional relations for centred cells can be derived easily from the table.

(iv) *Location of the origin* of the plane group with respect to the unit cell of the space group. The same description is used as for the location of symmetry elements (*cf.* Section 2.2.9).

Example
  'Origin at x, 0, 0' or 'Origin at $\frac{1}{4}, \frac{1}{4}, z$'.

2.2.14.2. *Projections of centred cells (lattices)*

For centred lattices, two different cases may occur:

(i) The projection direction is parallel to a lattice-centring vector. In this case, the projected plane cell is primitive for the centring types A, B, C, I and R. For F lattices, the multiplicity is reduced from 4 to 2 because c-centred plane cells result from projections along face diagonals of three-dimensional F cells.

Examples
(1) A body-centred lattice with centring vector $\frac{1}{2}(\mathbf{a} + \mathbf{b} + \mathbf{c})$ gives a primitive net, if projected along $[111]$, $[\bar{1}1\bar{1}]$, $[1\bar{1}\bar{1}]$ or $[\bar{1}1\bar{1}]$.
(2) A C-centred lattice projects to a primitive net along the directions $[110]$ and $[1\bar{1}0]$.
(3) An R-centred lattice described with 'hexagonal axes' (triple cell) results in a primitive net, if projected along $[\bar{1}11]$, $[211]$ or $[\bar{1}\bar{2}1]$ for the obverse setting. For the reverse setting, the corresponding directions are $[11\bar{1}]$, $[\bar{2}1\bar{1}]$, $[121]$; *cf.* Chapter 1.2.

(ii) The projection direction is not parallel to a lattice-centring vector (general projection direction). In this case, the plane cell has the same multiplicity as the three-dimensional cell. Usually, however, this centred plane cell is unconventional and a transformation is required to obtain the conventional plane cell. This transformation has been carried out for the projection data in this volume.

Examples
(1) Projection along $[010]$ of a cubic I-centred cell leads to an unconventional quadratic c-centred plane cell. A simple cell transformation leads to the conventional quadratic p cell.
(2) Projection along $[010]$ of an orthorhombic I-centred cell leads to a rectangular c-centred plane cell, which is conventional.
(3) Projection along $[001]$ of an R-centred cell (both in obverse and reverse setting) results in a triple hexagonal plane cell h (the two-dimensional analogue of the H cell, *cf.* Chapter 1.2). A simple cell transformation leads to the conventional hexagonal p cell.

2.2.14.3. *Projections of symmetry elements*

A symmetry element of a space group does not project as a symmetry element unless its orientation bears a special relation to the projection direction; all translation components of a symmetry

Table 2.2.14.2. *Projections of crystallographic symmetry elements*

Symmetry element in three dimensions	Symmetry element in projection
Arbitrary orientation	
Symmetry centre $\bar{1}$ Rotoinversion axis $\bar{3} \equiv 3 \times \bar{1}$	Rotation point 2 (at projection of centre)
Parallel to projection direction	
Rotation axis 2; 3; 4; 6	Rotation point 2; 3; 4; 6
Screw axis 2_1	Rotation point 2
$3_1, 3_2$	3
$4_1, 4_2, 4_3$	4
$6_1, 6_2, 6_3, 6_4, 6_5$	6
Rotoinversion axis $\bar{4}$	Rotation point 4
$\bar{6} \equiv 3/m$	3, with overlap of atoms
$\bar{3} \equiv 3 \times \bar{1}$	6
Reflection plane m	Reflection line m
Glide plane with $\perp$ component*	Glide line g
Glide plane without $\perp$ component*	Reflection line m
Normal to projection direction	
Rotation axis 2; 4; 6	Reflection line m
3	None
Screw axis 4_2; $6_2, 6_4$	Reflection line m
2_1; $4_1, 4_3$; $6_1, 6_3, 6_5$	Glide line g
$3_1, 3_2$	None
Rotoinversion axis $\bar{4}$	Reflection line m parallel to axis
$\bar{6} \equiv 3/m$	Reflection line m perpendicular to axis (through projection of inversion point)
$\bar{3} \equiv 3 \times \bar{1}$	Rotation point 2 (at projection of centre)
Reflection plane m	None, but overlap of atoms
Glide plane with glide vector $\mathbf{t}$	Translation with translation vector $\mathbf{t}$

* The term 'with $\perp$ component' refers to the component of the glide vector normal to the projection direction.

operation along the projection direction vanish, whereas those perpendicular to the projection direction (*i.e.* parallel to the plane of projection) may be retained. This is summarized in Table 2.2.14.2 for the various crystallographic symmetry elements. From this table the following conclusions can be drawn:

(i) *n*-fold rotation axes and *n*-fold screw axes, as well as rotoinversion axes $\bar{4}$, *parallel to the projection direction* project as *n*-fold rotation points; a $\bar{3}$ axis projects as a sixfold, a $\bar{6}$ axis as a threefold rotation point. For the latter, a doubling of the projected electron density occurs owing to the mirror plane normal to the projection direction ($\bar{6} \equiv 3/m$).

(ii) *n*-fold rotation axes and *n*-fold screw axes *normal to the projection direction* (*i.e.* parallel to the plane of projection) do not project as symmetry elements if *n* is odd. If *n* is even, all rotation and rotoinversion axes project as mirror lines: the same applies to the screw axes $4_2, 6_2$ and 6_4 because they contain an axis 2. Screw axes $2_1, 4_1, 4_3, 6_1, 6_3$ and 6_5 project as glide lines because they contain 2_1.

(iii) Reflection planes *normal* to the projection direction do not project as symmetry elements but lead to a doubling of the projected electron density owing to overlap of atoms. Projection of a glide plane results in an additional translation; the new translation vector

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is equal to the glide vector of the glide plane. Thus, a reduction of the translation period in that particular direction takes place.

(iv) Reflection planes *parallel* to the projection direction project as reflection lines. Glide planes project as glide lines or as reflection lines, depending upon whether the glide vector has or has not a component parallel to the projection plane.

(v) Centres of symmetry, as well as $\bar{3}$ axes in *arbitrary* orientation, project as twofold rotation points.

*Example: C*12/*c*1 (15, *b* unique, cell choice 1)

The *C*-centred cell has lattice points at 0, 0, 0 and $\frac{1}{2}, \frac{1}{2}, 0$. In all projections, the centre $\bar{1}$ projects as a twofold rotation point. Projection along [001]: The plane cell is centred; 2 ∥ [010] projects as *m*; the glide component $(0, 0, \frac{1}{2})$ of glide plane *c* vanishes and thus *c* projects as *m*.

Result: Plane group *c*2*mm* (9), $\mathbf{a}' = \mathbf{a}_p, \mathbf{b}' = \mathbf{b}$.

Projection along [100]: The periodicity along *b* is halved because of the *C* centring; 2 ∥ [010] projects as *m*; the glide component $(0, 0, \frac{1}{2})$ of glide plane *c* is retained and thus *c* projects as *g*.

Result: Plane group *p*2*gm* (7), $\mathbf{a}' = \mathbf{b}/2, \ \mathbf{b}' = \mathbf{c}_p$.

Projection along [010]: The periodicity along *a* is halved because of the *C* centring; that along *c* is halved owing to the glide component $(0, 0, \frac{1}{2})$ of glide plane *c*; 2 ∥ [010] projects as 2.

Result: Plane group *p*2 (2), $\mathbf{a}' = \mathbf{c}/2, \mathbf{b}' = \mathbf{a}/2$.

Further details about the geometry of projections can be found in publications by Buerger (1965) and Biedl (1966).

2.2.15. Maximal subgroups and minimal supergroups

The present section gives a brief summary, without theoretical explanations, of the sub- and supergroup data in the space-group tables. The theoretical background is provided in Section 8.3.3 and Part 13. Detailed sub- and supergroup data are given in *International Tables for Crystallography* Volume A1 (2004).

2.2.15.1. *Maximal non-isomorphic subgroups**

The maximal non-isomorphic subgroups $\mathcal{H}$ of a space group $\mathcal{G}$ are divided into two types:

> **I** *translationengleiche* or *t* subgroups
>
> **II** *klassengleiche* or *k* subgroups.

For practical reasons, type **II** is subdivided again into two blocks:

IIa the conventional cells of $\mathcal{G}$ and $\mathcal{H}$ are the same

IIb the conventional cell of $\mathcal{H}$ is larger than that of $\mathcal{G}$. †

Block **IIa** has no entries for space groups $\mathcal{G}$ with a primitive cell. For space groups $\mathcal{G}$ with a centred cell, it contains those maximal subgroups $\mathcal{H}$ that have lost some or all centring translations of $\mathcal{G}$ but none of the integral translations ('decentring' of a centred cell).

Within each block, the subgroups are listed in order of increasing index [*i*] and in order of decreasing space-group number for each value of *i*.

(i) *Blocks* **I** *and* **IIa**

In blocks **I** and **IIa**, *every* maximal subgroup $\mathcal{H}$ of a space group $\mathcal{G}$ is listed with the following information:

[*i*] HMS1 (HMS2, No.) Sequence of numbers.

_____

* Space groups with different space-group numbers are non-isomorphic, except for the members of the 11 pairs of enantiomorphic space groups which are isomorphic.
† Subgroups belonging to the enantiomorphic space-group type of $\mathcal{G}$ are isomorphic to $\mathcal{G}$ and, therefore, are listed under **IIc** and not under **IIb**.

The symbols have the following meaning:

[*i*]: index of $\mathcal{H}$ in $\mathcal{G}$ (*cf.* Section 8.1.6, footnote);

HMS1: Hermann–Mauguin symbol of $\mathcal{H}$, referred to the coordinate system and setting of $\mathcal{G}$; this symbol may be unconventional;

(HMS2, No.): conventional short Hermann–Mauguin symbol of $\mathcal{H}$, given only if HMS1 is not in conventional short form, and the space-group number of $\mathcal{H}$.

Sequence of numbers: coordinate triplets of $\mathcal{G}$ retained in $\mathcal{H}$. The numbers refer to the numbering scheme of the coordinate triplets of the general position of $\mathcal{G}$ (*cf.* Section 2.2.9). The following abbreviations are used:

Block **I** (all translations retained):

Number +	Coordinate triplet given by *Number*, plus those obtained by adding all centring translations of $\mathcal{G}$.
(*Numbers*) +	The same, but applied to all *Numbers* between parentheses.

Block **IIa** (not all translations retained):

Number + (t_1, t_2, t_3)	Coordinate triplet obtained by adding the translation t_1, t_2, t_3 to the triplet given by *Number*.
(*Numbers*) + (t_1, t_2, t_3)	The same, but applied to all *Numbers* between parentheses.

In blocks **I** and **IIa**, sets of conjugate subgroups are linked by left-hand braces. For an example, see space group $R\bar{3}$ (148) below.

Examples

(1) $\mathcal{G}$: *C*1*m*1 (8)

I	[2] *C*1 (*P*1, 1)	1+
IIa	[2] *P*1*a*1 (*Pc*, 7)	1; 2 + (1/2, 1/2, 0)
	[2] *P*1*m*1 (*Pm*, 6)	1; 2

where the numbers have the following meaning:

1+	x, y, z; $\quad x + 1/2, y + 1/2, z$
1; 2	x, y, z; $\quad x, \bar{y}, z$
1; 2 + (1/2, 1/2, 0)	x, y, z; $\quad x + 1/2, \bar{y} + 1/2, z$.

(2) $\mathcal{G}$: *Fdd*2 (43)

I [2] *F*112 (*C*2, 5) $\qquad$ (1; 2)+

where the numbers have the following meaning:

$$(1; 2)+ \quad x, y, z; \quad x + 1/2, y + 1/2, z;$$
$$x + 1/2, y, z + 1/2; \quad x, y + 1/2, z + 1/2;$$
$$\bar{x}, \bar{y}, z; \quad \bar{x} + 1/2, \bar{y} + 1/2, z;$$
$$\bar{x} + 1/2, \bar{y}, z + 1/2; \quad \bar{x}, \bar{y} + 1/2, z + 1/2.$$

(3) $\mathcal{G}$: $P4_2/nmc = P4_2/n2_1/m2/c$ (137)

I [2] $P2/n2_1/m1$ (*Pmmn*, 59) 1; 2; 5; 6; 9; 10; 13; 14.

Operations $4_2, 2$ and *c*, occurring in the Hermann–Mauguin symbol of $\mathcal{G}$, are lacking in $\mathcal{H}$. In the unconventional 'tetragonal version' $P2/n2_1/m1$ of the symbol of $\mathcal{H}$, $2_1/m$ stands for two sets of $2_1/m$ (along the two orthogonal secondary symmetry directions), implying that $\mathcal{H}$ is orthorhombic. In the conventional 'orthorhombic version', the full symbol of $\mathcal{H}$ reads $P2_1/m2_1/m2/n$ and the short symbol *Pmmn*.