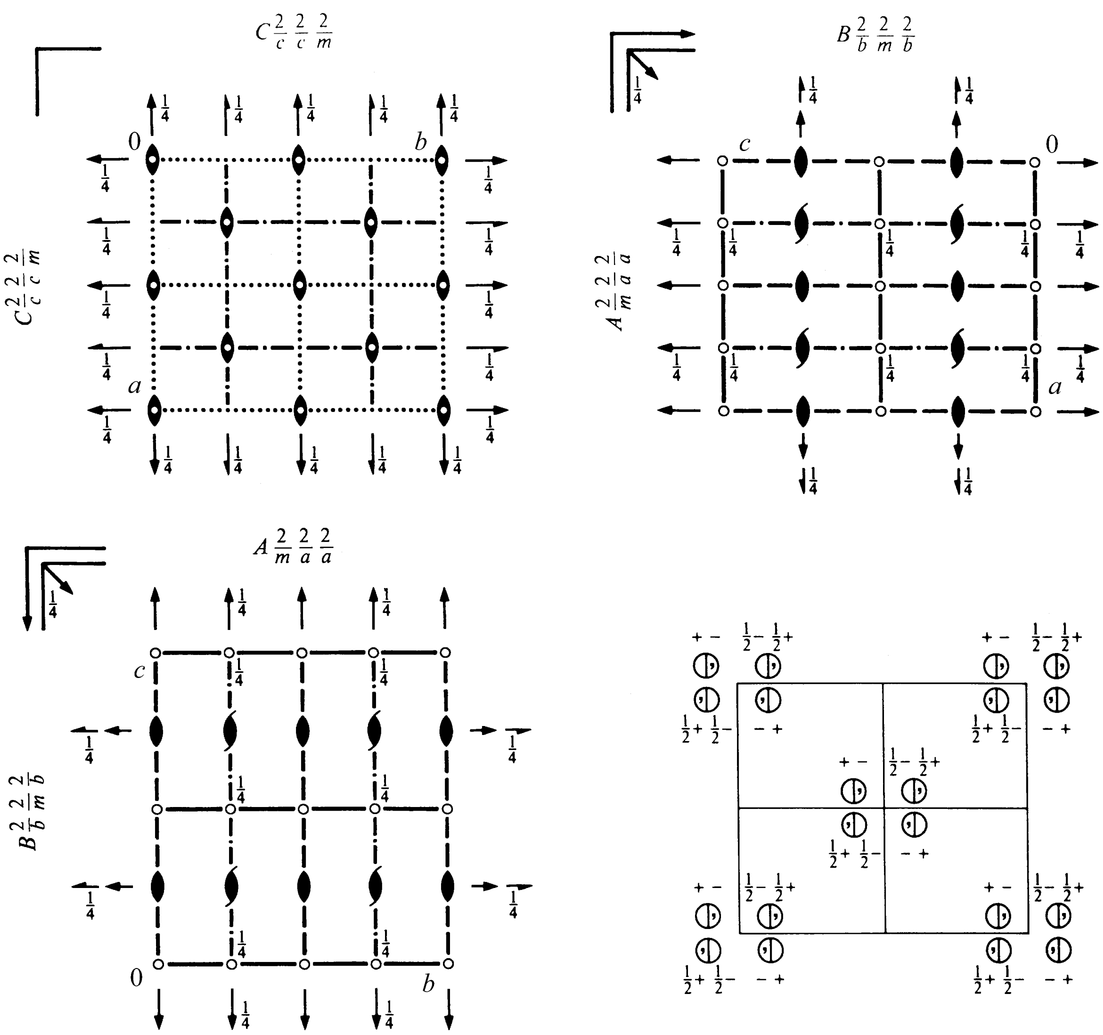
① $Cccm$ D_{2h}^{20} mmm Orthorhombic

② No. 66 $C\ 2/c\ 2/c\ 2/m$ Patterson symmetry $Cmmm$

③



④ **Origin** at centre ($2/m$) at $cc2/m$

⑤ **Asymmetric unit** $0 \le x \le \frac{1}{4};\quad 0 \le y \le \frac{1}{2};\quad 0 \le z \le \frac{1}{2}$

⑥ **Symmetry operations**

For $(0,0,0)+$ set

(1) 1	(2) $2\quad 0,0,z$	(3) $2\quad 0,y,\frac{1}{4}$	(4) $2\quad x,0,\frac{1}{4}$
(5) $\bar{1}\quad 0,0,0$	(6) $m\quad x,y,0$	(7) $c\quad x,0,z$	(8) $c\quad 0,y,z$

For $(\frac{1}{2},\frac{1}{2},0)+$ set

(1) $t(\frac{1}{2},\frac{1}{2},0)$	(2) $2\quad \frac{1}{4},\frac{1}{4},z$	(3) $2(0,\frac{1}{2},0)\quad \frac{1}{4},y,\frac{1}{4}$	(4) $2(\frac{1}{2},0,0)\quad x,\frac{1}{4},\frac{1}{4}$
(5) $\bar{1}\quad \frac{1}{4},\frac{1}{4},0$	(6) $n(\frac{1}{2},\frac{1}{2},0)\quad x,y,0$	(7) $n(\frac{1}{2},0,\frac{1}{2})\quad x,\frac{1}{4},z$	(8) $n(0,\frac{1}{2},\frac{1}{2})\quad \frac{1}{4},y,z$

EXPLANATION OF THE SPACE-GROUP DATA

Headline: Section 2.1.3.3. The headline of each plane-group or space-group table consists of two (sometimes three) lines which contain the following information:

① First line:

Short international (Hermann–Mauguin) symbol for the plane or space group: Sections 1.4.1 and 2.1.3.4, and Chapter 3.3.

Schoenflies symbol for the space group: Section 1.4.1 and Chapter 3.3. No Schoenflies symbols exist for the plane groups.

Crystal class: The short international (Hermann–Mauguin) symbol for the point group to which the plane or space group belongs (*cf.* Section 1.4.1 and Chapter 3.3).

The name of the *crystal system* to which the plane or space group belongs (Section 1.3.4.4, *cf.* Table 2.1.1.1). There exist four crystal systems in two-dimensional space (oblique, rectangular, square, hexagonal) and seven crystal systems in three-dimensional space (triclinic, monoclinic, orthorhombic, tetragonal, trigonal, hexagonal and cubic).

② Second line:

The *sequential number of the plane or space group*, as introduced in *International Tables for X-ray Crystallography* Vol. I (1952) (*cf.* Section 1.4.1.2).

The *full Hermann–Mauguin symbol* for the plane or space group: Sections 1.4.1 and 2.1.3.4, and Chapter 3.3.

Patterson symmetry: Section 2.1.3.5. The *Patterson symmetry* is a crystallographic space group denoted by its Hermann–Mauguin symbol. The Patterson symmetry has the same Bravais-lattice type as the space group itself, while the 'point-group part' of the Patterson-symmetry symbol represents the Laue class to which the plane group or space group belongs.

The third line of the headline is used, where appropriate, to indicate origin choices, settings, cell choices and coordinate axes (see Section 2.1.3.2).

③ *Space-group diagrams*, consisting of one or several orthogonal projections which show the relative location and orientation of the symmetry elements, and one illustration of a set of symmetry-equivalent points in general position. The numbers and types of the diagrams depend on the crystal system. The diagrams and their coordinate axes are described in Section 2.1.3.6; the graphical symbols of the symmetry elements are listed in Tables 2.1.2.2 to 2.1.2.7.

④ *Origin* of the unit cell: Section 2.1.3.7. In the line *Origin*, the site symmetry of the origin is stated, if different from the identity. A further symbol indicates all symmetry elements (including glide planes and screw axes) that pass through the origin, if any. For noncentrosymmetric space groups, the origin is at a point of highest site symmetry. All centrosymmetric space groups are described with an inversion centre as origin. A further description is given if a centrosymmetric space group contains points of high site symmetry that do not coincide with a centre of symmetry. For space groups with two origin choices, for each of the two origins the location relative to the other origin is also given.

⑤ *Asymmetric unit*: Section 2.1.3.8. An asymmetric unit of a space group is a (simply connected) smallest closed part of space from which, by application of all symmetry operations of the space group, the whole of space is filled. The choice of the asymmetric unit is not unique – it may depend on its intended use. In the space-group tables of this volume the asymmetric units are chosen in such a way that Fourier summations can be performed conveniently.

⑥ *Symmetry operations*: Sections 1.4.2.1 and 2.1.3.9, and Chapter 1.2. For each point $\tilde{x}, \tilde{y}, \tilde{z}$ of the general position, the symmetry operation is listed that transforms the initial point x, y, z into the point under consideration. The symbol of the symmetry operation describes the nature of the operation, its glide or screw component (given between parentheses), if present, and the location and orientation of the corresponding geometric element. The symmetry operations are numbered in the same way as the corresponding coordinate triplets of the general position. For space groups with centred cells, several blocks of *Symmetry operations* correspond to the one *General position* block: the number of blocks equals the multiplicity of the centred cell and the numbering scheme of the general position is applied in each block.

EXPLANATION OF THE SPACE-GROUP DATA

① Headline in abbreviated form:

The *sequential number of the plane or space group*, as introduced in *International Tables for X-ray Crystallography* Vol. I (1952) (*cf.* Section 1.4.1.2).

Short international (Hermann–Mauguin) symbol for the plane or space group: Sections 1.4.1 and 2.1.3.4, and Chapter 3.3.

② *Generators selected*: Sections 1.4.3 and 2.1.3.10. The line *Generators selected* states the symmetry operations and their sequence, selected to generate all symmetry-equivalent points of the *General position* from a point with coordinates x, y, z. The generating translations are listed explicitly, while the non-translational generators are given as numbers (p) that refer to the coordinate triplets of the general position and the corresponding entries under *Symmetry operations*.

③ *Positions*: Sections 1.4.4 and 2.1.3.11. The entries under *Positions* (called also *Wyckoff positions*) consist of the block *General position* given at the top followed downwards by the blocks of various special Wyckoff positions with decreasing multiplicity and increasing site symmetry. For each general and special position its multiplicity, Wyckoff letter, oriented site-symmetry symbol, the appropriate coordinate triplets and the reflection conditions are listed:

Multiplicity of the Wyckoff position: this is the number of symmetry-equivalent points that lie in the conventional unit cell. The quotient of the multiplicity for the general position by that of a special position gives the order of the site-symmetry group of the special position.

Wyckoff letter: Each Wyckoff position is labelled by a letter in alphabetical order, starting with '*a*' for a position with site-symmetry group of maximal order and ending with the highest letter for the general position.

Oriented site-symmetry symbol (third column): the site symmetry at the points of a special position is described by the site-symmetry group, which is isomorphic to a subgroup of the point group of the space group. The site-symmetry groups are indicated by *oriented site-symmetry symbols* that show how the symmetry elements at a site are related to the symmetry elements of the crystal lattice (*cf.* Section 2.1.3.12).

Coordinates: The coordinate triplets of a position represent the coordinates of the symmetry-equivalent points in the unit cell. The sequence of coordinate triplets is produced in the same order as the symmetry operations, generated by the chosen set of generators, omitting duplicates. For centred space groups, the centring translations have to be added to the listed coordinate triplets in order to obtain a complete set of triplets for the Wyckoff position.

The coordinate triplets of the general position can also be interpreted as a shorthand form of the matrix representation of the symmetry operations of the space group specified up to translations (*cf.* Sections 1.3.3.2 and 1.4.2.3).

Reflection conditions (last column): Sections 1.6.3 and 2.1.3.13. The listed systematic reflection conditions for diffraction of radiation by crystals are formulated as 'conditions of occurrence' (structure factor not systematically zero). The *General conditions* are associated with systematic absences caused by the presence of lattice centrings, screw axes and glide planes. The *Special conditions* (or 'extra' conditions) apply only to special Wyckoff positions and always occur in addition to the general conditions of the space group.

④ *Symmetry of special projections*: Sections 1.4.5.3 and 2.1.3.14. For each space group, orthogonal projections along three (symmetry) directions are listed. Given are the projection direction, the Hermann–Mauguin symbol of the plane group of the projection, the relations between the basis vectors of the plane group and the basis vectors of the space group, and the location of the origin of the plane group with respect to the unit cell of the space group.

EXPLANATION OF THE SPACE-GROUP DATA

② **Generators selected** (1); $t(1,0,0)$; $t(0,1,0)$; $t(0,0,1)$; $t(\frac{1}{2},\frac{1}{2},0)$; (2); (3); (5)

③ **Positions**

Multiplicity	Wyckoff letter	Site symmetry	Coordinates $(0,0,0)+$ $(\frac{1}{2},\frac{1}{2},0)+$				Reflection conditions
							General:
16	m	1	(1) x,y,z	(2) $\bar{x},\bar{y},z$	(3) $\bar{x},y,\bar{z}+\frac{1}{2}$	(4) $x,\bar{y},\bar{z}+\frac{1}{2}$	hkl: $h+k=2n$
			(5) $\bar{x},\bar{y},\bar{z}$	(6) $x,y,\bar{z}$	(7) $x,\bar{y},z+\frac{1}{2}$	(8) $\bar{x},y,z+\frac{1}{2}$	$0kl$: $k,l=2n$
							$h0l$: $h,l=2n$
							$hk0$: $h+k=2n$
							$h00$: $h=2n$
							$0k0$: $k=2n$
							$00l$: $l=2n$
							Special: as above, plus
8	l	$..m$	$x,y,0$	$\bar{x},\bar{y},0$	$\bar{x},y,\frac{1}{2}$	$x,\bar{y},\frac{1}{2}$	no extra conditions
8	k	$..2$	$\frac{1}{4},\frac{1}{4},z$	$\frac{3}{4},\frac{1}{4},\bar{z}+\frac{1}{2}$	$\frac{3}{4},\frac{3}{4},\bar{z}$	$\frac{1}{4},\frac{3}{4},z+\frac{1}{2}$	hkl: $k+l=2n$
8	j	$..2$	$0,\frac{1}{2},z$	$0,\frac{1}{2},\bar{z}+\frac{1}{2}$	$0,\frac{1}{2},\bar{z}$	$0,\frac{1}{2},z+\frac{1}{2}$	hkl: $l=2n$
8	i	$..2$	$0,0,z$	$0,0,\bar{z}+\frac{1}{2}$	$0,0,\bar{z}$	$0,0,z+\frac{1}{2}$	hkl: $l=2n$
8	h	$.2.$	$0,y,\frac{1}{4}$	$0,\bar{y},\frac{1}{4}$	$0,\bar{y},\frac{3}{4}$	$0,y,\frac{3}{4}$	hkl: $l=2n$
8	g	$2..$	$x,0,\frac{1}{4}$	$\bar{x},0,\frac{1}{4}$	$\bar{x},0,\frac{3}{4}$	$x,0,\frac{3}{4}$	hkl: $l=2n$
4	f	$..2/m$	$\frac{1}{4},\frac{3}{4},0$	$\frac{3}{4},\frac{3}{4},\frac{1}{2}$			hkl: $k+l=2n$
4	e	$..2/m$	$\frac{1}{4},\frac{1}{4},0$	$\frac{3}{4},\frac{1}{4},\frac{1}{2}$			hkl: $k+l=2n$
4	d	$..2/m$	$0,\frac{1}{2},0$	$0,\frac{1}{2},\frac{1}{2}$			hkl: $l=2n$
4	c	$..2/m$	$0,0,0$	$0,0,\frac{1}{2}$			hkl: $l=2n$
4	b	222	$0,\frac{1}{2},\frac{1}{4}$	$0,\frac{1}{2},\frac{3}{4}$			hkl: $l=2n$
4	a	222	$0,0,\frac{1}{4}$	$0,0,\frac{3}{4}$			hkl: $l=2n$

④ **Symmetry of special projections**

Along [001] $c2mm$
$\mathbf{a}'=\mathbf{a}$ $\mathbf{b}'=\mathbf{b}$
Origin at $0,0,z$

Along [100] $p2mm$
$\mathbf{a}'=\frac{1}{2}\mathbf{b}$ $\mathbf{b}'=\frac{1}{2}\mathbf{c}$
Origin at $x,0,0$

Along [010] $p2mm$
$\mathbf{a}'=\frac{1}{2}\mathbf{c}$ $\mathbf{b}'=\frac{1}{2}\mathbf{a}$
Origin at $0,y,0$

EXPLANATION OF THE SPACE-GROUP DATA