

- ① *Headline* in abbreviated form.
- ② *Generators selected*: Sections 2.2.10 and 8.3.5. A set of generators, as selected for these *Tables*, is listed in the form of translations and numbers of general-position coordinates. The generators determine the sequence of the coordinate triplets in the general position and of the corresponding symmetry operations.
- ③ *Positions*: Sections 2.2.11 and 8.3.2. The general Wyckoff position is given at the top, followed downwards by the 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, as well as the appropriate coordinate triplets and the reflection conditions, are listed. The coordinate triplets of the general position are numbered sequentially; *cf. Symmetry operations*.

Oriented site-symmetry symbol (third column): Section 2.2.12. The site symmetry at the points of a special position is given in oriented form.

Reflection conditions (right-most column): Section 2.2.13.

[*Lattice complexes* are described in Part 14; Tables 14.2.3.1 and 14.2.3.2 show the assignment of Wyckoff positions to Wyckoff sets and to lattice complexes.]

- ④ *Symmetry of special projections*: Section 2.2.14. For each space group, orthographic projections along three (symmetry) directions are listed. Given are the projection direction, the plane group of the projection, as well as the axes and the origin of the projected cell.
- ⑤ *Maximal non-isomorphic subgroups*: Sections 2.2.15 and 8.3.3.

Type **I**: *translationengleiche* or *t* subgroups;

Type **IIa**: *klassengleiche* or *k* subgroups, obtained by ‘decentring’ the conventional cell; applies only to space groups with centred cells;

Type **IIb**: *klassengleiche* or *k* subgroups, obtained by enlarging the conventional cell.

Given are:

For types **I** and **IIa**: Index [between brackets]; ‘unconventional’ Hermann–Mauguin symbol of the subgroup; ‘conventional’ Hermann–Mauguin symbol of the subgroup, if different (between parentheses); coordinate triplets retained in subgroup.

For type **IIb**: Index [between brackets]; ‘unconventional’ Hermann–Mauguin symbol of the subgroup; basis-vector relations between group and subgroup (between parentheses); ‘conventional’ Hermann–Mauguin symbol of the subgroup, if different (between parentheses).

- ⑥ *Maximal isomorphic subgroups of lowest index*: Sections 2.2.15, 8.3.3 and 13.1.2.

Type **IIc**: *klassengleiche* or *k* subgroups of lowest index which are of the same type as the group, *i.e.* have the same standard Hermann–Mauguin symbol. Data as for subgroups of type **IIb**.

- ⑦ *Minimal non-isomorphic supergroups*: Sections 2.2.15 and 8.3.3.

The list contains the reverse relations of the subgroup tables; only types **I** (*t* supergroups) and **II** (*k* supergroups) are distinguished. Data as for subgroups of type **IIb**.

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)

③ **Positions**

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

④ **Symmetry of special projections**

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

Along [100] $p1m1$
 $\mathbf{a}' = \frac{1}{2}\mathbf{b}$ $\mathbf{b}' = \mathbf{c}$
Origin at $x,0,0$

Along [010] $p11m$
 $\mathbf{a}' = \mathbf{c}$ $\mathbf{b}' = \frac{1}{2}\mathbf{a}$
Origin at $0,y,0$

⑤ **Maximal non-isomorphic subgroups**

I [2] $C1m1(Cm, 8)$ (1; 3)+
[2] $Cm11(Cm, 8)$ (1; 4)+
[2] $C112(P2, 3)$ (1; 2)+

IIa [2] $Pba2(32)$ 1; 2; (3; 4) + $(\frac{1}{2}, \frac{1}{2}, 0)$
[2] $Pbm2(Pma2, 28)$ 1; 3; (2; 4) + $(\frac{1}{2}, \frac{1}{2}, 0)$
[2] $Pma2(28)$ 1; 4; (2; 3) + $(\frac{1}{2}, \frac{1}{2}, 0)$
[2] $Pmm2(25)$ 1; 2; 3; 4

IIb [2] $Ima2(\mathbf{c}' = 2\mathbf{c})$ (46); [2] $IBM2(\mathbf{c}' = 2\mathbf{c})$ ($Ima2, 46$); [2] $Iba2(\mathbf{c}' = 2\mathbf{c})$ (45); [2] $Imm2(\mathbf{c}' = 2\mathbf{c})$ (44); [2] $Ccc2(\mathbf{c}' = 2\mathbf{c})$ (37);
[2] $Cmc2_1(\mathbf{c}' = 2\mathbf{c})$ (36); [2] $Ccm2_1(\mathbf{c}' = 2\mathbf{c})$ ($Cmc2_1, 36$)

⑥ **Maximal isomorphic subgroups of lowest index**

IIc [2] $Cmm2(\mathbf{c}' = 2\mathbf{c})$ (35); [3] $Cmm2(\mathbf{a}' = 3\mathbf{a} \text{ or } \mathbf{b}' = 3\mathbf{b})$ (35)

⑦ **Minimal non-isomorphic supergroups**

I [2] $Cmmm(65)$; [2] $Cmme(67)$; [2] $P4mm(99)$; [2] $P4bm(100)$; [2] $P4_{2}cm(101)$; [2] $P4_{2}nm(102)$; [2] $P\bar{4}2m(111)$;
[2] $P\bar{4}2_1m(113)$; [3] $P6mm(183)$

II [2] $Fmm2(42)$; [2] $Pmm2(\mathbf{a}' = \frac{1}{2}\mathbf{a}, \mathbf{b}' = \frac{1}{2}\mathbf{b})$ (25)