

$P\bar{4}$

No. 81

$P\bar{4}$

$S_4^1$

**Generators selected** (1);  $t(1,0,0)$ ;  $t(0,1,0)$ ;  $t(0,0,1)$ ; (2); (3)

**General position**

Multiplicity,  
Wyckoff letter,  
Site symmetry

Coordinates

4  $h$  1

(1)  $x, y, z$  (2)  $\bar{x}, \bar{y}, z$  (3)  $y, \bar{x}, \bar{z}$  (4)  $\bar{y}, x, \bar{z}$

**I Maximal translationengleiche subgroups**

[2]  $P2$  (3,  $P112$ ) 1; 2

**II Maximal klassengleiche subgroups**

• **Enlarged unit cell**

[2]  $\mathbf{c}' = 2\mathbf{c}$

$P\bar{4}$  (81)  $\langle 2; 3 \rangle$

$\mathbf{a}, \mathbf{b}, 2\mathbf{c}$

$P\bar{4}$  (81)  $\langle 2; 3 + (0, 0, 1) \rangle$

$\mathbf{a}, \mathbf{b}, 2\mathbf{c}$

0, 0, 1/2

[2]  $\mathbf{a}' = 2\mathbf{a}, \mathbf{b}' = 2\mathbf{b}$

$C\bar{4}$  (81,  $P\bar{4}$ )  $\langle 2; 3 \rangle$

$\mathbf{a} - \mathbf{b}, \mathbf{a} + \mathbf{b}, \mathbf{c}$

$C\bar{4}$  (81,  $P\bar{4}$ )  $\langle 2 + (1, 1, 0); 3 + (0, 1, 0) \rangle$

$\mathbf{a} - \mathbf{b}, \mathbf{a} + \mathbf{b}, \mathbf{c}$

1/2, 1/2, 0

[2]  $\mathbf{a}' = 2\mathbf{a}, \mathbf{b}' = 2\mathbf{b}, \mathbf{c}' = 2\mathbf{c}$

$F\bar{4}$  (82,  $I\bar{4}$ )  $\langle 2; 3 \rangle$

$\mathbf{a} - \mathbf{b}, \mathbf{a} + \mathbf{b}, 2\mathbf{c}$

$F\bar{4}$  (82,  $I\bar{4}$ )  $\langle 2; 3 + (0, 0, 1) \rangle$

$\mathbf{a} - \mathbf{b}, \mathbf{a} + \mathbf{b}, 2\mathbf{c}$

0, 0, 1/2

[3]  $\mathbf{c}' = 3\mathbf{c}$

$P\bar{4}$  (81)  $\langle 2; 3 \rangle$

$\mathbf{a}, \mathbf{b}, 3\mathbf{c}$

$P\bar{4}$  (81)  $\langle 2; 3 + (0, 0, 2) \rangle$

$\mathbf{a}, \mathbf{b}, 3\mathbf{c}$

0, 0, 1

$P\bar{4}$  (81)  $\langle 2; 3 + (0, 0, 4) \rangle$

$\mathbf{a}, \mathbf{b}, 3\mathbf{c}$

0, 0, 2

• **Series of maximal isomorphic subgroups**

[ $p$ ]  $\mathbf{c}' = p\mathbf{c}$

$P\bar{4}$  (81)  $\langle 2; 3 + (0, 0, 2u) \rangle$

$\mathbf{a}, \mathbf{b}, p\mathbf{c}$

0, 0,  $u$

$p > 2; 0 \leq u < p$

$p$  conjugate subgroups for the prime  $p$

[ $p^2$ ]  $\mathbf{a}' = p\mathbf{a}, \mathbf{b}' = p\mathbf{b}$

$P\bar{4}$  (81)  $\langle 2 + (2u, 2v, 0); 3 + (u - v, u + v, 0) \rangle$

$p\mathbf{a}, p\mathbf{b}, \mathbf{c}$

$u, v, 0$

$p > 2; 0 \leq u < p; 0 \leq v < p$

$p^2$  conjugate subgroups for prime  $p \equiv 3 \pmod{4}$

[ $p = q^2 + r^2$ ]  $\mathbf{a}' = q\mathbf{a} - r\mathbf{b}, \mathbf{b}' = r\mathbf{a} + q\mathbf{b}$

$P\bar{4}$  (81)  $\langle 2 + (2u, 0, 0); 3 + (u, u, 0) \rangle$

$q\mathbf{a} - r\mathbf{b}, r\mathbf{a} + q\mathbf{b}, \mathbf{c}$

$u, 0, 0$

$q > 0; r > 0; p > 4; 0 \leq u < p$

$p$  conjugate subgroups for prime  $p \equiv 1 \pmod{4}$

**I Minimal translationengleiche supergroups**

[2]  $P4/m$  (83); [2]  $P4_2/m$  (84); [2]  $P4/n$  (85); [2]  $P4_2/n$  (86); [2]  $P\bar{4}2m$  (111); [2]  $P\bar{4}2c$  (112); [2]  $P\bar{4}2_1m$  (113); [2]  $P\bar{4}2_1c$  (114);

[2]  $P\bar{4}m2$  (115); [2]  $P\bar{4}c2$  (116); [2]  $P\bar{4}b2$  (117); [2]  $P\bar{4}n2$  (118)

**II Minimal non-isomorphic klassengleiche supergroups**

• **Additional centring translations**

[2]  $I\bar{4}$  (82)

• **Decreased unit cell**

none