

D_{4h}^6
 $P4/m2_1/n2/c$

No. 128

 $P4/mnc$
Generators selected (1); $t(1,0,0)$; $t(0,1,0)$; $t(0,0,1)$; (2); (3); (5); (9)

General position

 Multiplicity,
Wyckoff letter,
Site symmetry

Coordinates

| | | | | | | |
|----|----------|---|---|---|--|---|
| 16 | <i>i</i> | 1 | (1) x, y, z | (2) \bar{x}, \bar{y}, z | (3) \bar{y}, x, z | (4) y, \bar{x}, z |
| | | | (5) $\bar{x} + \frac{1}{2}, y + \frac{1}{2}, \bar{z} + \frac{1}{2}$ | (6) $x + \frac{1}{2}, \bar{y} + \frac{1}{2}, \bar{z} + \frac{1}{2}$ | (7) $y + \frac{1}{2}, x + \frac{1}{2}, \bar{z} + \frac{1}{2}$ | (8) $\bar{y} + \frac{1}{2}, \bar{x} + \frac{1}{2}, \bar{z} + \frac{1}{2}$ |
| | | | (9) $\bar{x}, \bar{y}, \bar{z}$ | (10) x, y, \bar{z} | (11) y, \bar{x}, \bar{z} | (12) \bar{y}, x, \bar{z} |
| | | | (13) $x + \frac{1}{2}, \bar{y} + \frac{1}{2}, z + \frac{1}{2}$ | (14) $\bar{x} + \frac{1}{2}, y + \frac{1}{2}, z + \frac{1}{2}$ | (15) $\bar{y} + \frac{1}{2}, \bar{x} + \frac{1}{2}, z + \frac{1}{2}$ | (16) $y + \frac{1}{2}, x + \frac{1}{2}, z + \frac{1}{2}$ |

I Maximal translationengleiche subgroups

| | | | |
|--------------------------------|----------------------------|------------------------|-------------|
| [2] $P\bar{4}n2$ (118) | 1; 2; 7; 8; 11; 12; 13; 14 | | |
| [2] $P4_2c$ (114) | 1; 2; 5; 6; 11; 12; 15; 16 | | |
| [2] $P4nc$ (104) | 1; 2; 3; 4; 13; 14; 15; 16 | | |
| [2] $P4_22$ (90) | 1; 2; 3; 4; 5; 6; 7; 8 | | 0, 1/2, 1/4 |
| [2] $P4/m11$ (83, $P4/m$) | 1; 2; 3; 4; 9; 10; 11; 12 | | |
| [2] $P2/m12/c$ (66, $Cccm$) | 1; 2; 7; 8; 9; 10; 15; 16 | a - b, a + b, c | 0, 1/2, 0 |
| [2] $P2/m2_1/n1$ (58, $Pnmm$) | 1; 2; 5; 6; 9; 10; 13; 14 | | |

II Maximal klassengleiche subgroups

• Enlarged unit cell

| | | | |
|---|--|-----------------|---------|
| [3] $\mathbf{c}' = 3\mathbf{c}$ | | | |
| $\left\{ \begin{array}{l} P4/mnc \text{ (128)} \\ P4/mnc \text{ (128)} \\ P4/mnc \text{ (128)} \end{array} \right.$ | $\langle 2; 3; 9; 5 + (0, 0, 1) \rangle$ | a, b, 3c | 0, 0, 1 |
| | $\langle 2; 3; 5 + (0, 0, 3); 9 + (0, 0, 2) \rangle$ | a, b, 3c | 0, 0, 2 |
| | $\langle 2; 3; 5 + (0, 0, 5); 9 + (0, 0, 4) \rangle$ | a, b, 3c | 0, 0, 2 |

• Series of maximal isomorphic subgroups

| | | | |
|--|---|------------------|----------------|
| [<i>p</i>] $\mathbf{c}' = p\mathbf{c}$ | | | |
| $P4/mnc$ (128) | $\langle 2; 3; 5 + (0, 0, \frac{p}{2} - \frac{1}{2} + 2u); 9 + (0, 0, 2u) \rangle$ $p > 2; 0 \leq u < p$ <i>p</i> conjugate subgroups for the prime <i>p</i> | a, b, pc | 0, 0, <i>u</i> |
| [<i>p</i> ²] $\mathbf{a}' = p\mathbf{a}, \mathbf{b}' = p\mathbf{b}$ | | | |
| $P4/mnc$ (128) | $\langle (2; 9) + (2u, 2v, 0); 3 + (u + v, -u + v, 0); 5 + (\frac{p}{2} - \frac{1}{2} + 2u, \frac{p}{2} - \frac{1}{2}, 0) \rangle$ $p > 2; 0 \leq u < p; 0 \leq v < p$ <i>p</i> ² conjugate subgroups for the prime <i>p</i> | pa, pb, c | <i>u, v, 0</i> |

I Minimal translationengleiche supergroups

none

II Minimal non-isomorphic klassengleiche supergroups

• Additional centring translations

 [2] $C4/mcc$ (124, $P4/mcc$); [2] $I4/mmm$ (139)

• Decreased unit cell

 [2] $\mathbf{c}' = \frac{1}{2}\mathbf{c}$ $P4/mbm$ (127)