

D_{4h}^1 $P4/m2/m2/m$

No. 123

 $P4/mmm$ 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 | u | 1 | (1) x, y, z | (2) \bar{x}, \bar{y}, z | (3) \bar{y}, x, z | (4) y, \bar{x}, z |
| | | | (5) \bar{x}, y, \bar{z} | (6) x, \bar{y}, \bar{z} | (7) y, x, \bar{z} | (8) $\bar{y}, \bar{x}, \bar{z}$ |
| | | | (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, \bar{y}, z | (14) \bar{x}, y, z | (15) \bar{y}, \bar{x}, z | (16) y, x, z |

I Maximal translationengleiche subgroups

| | | |
|------------------------------|----------------------------|-------------------|
| [2] $P4m2$ (115) | 1; 2; 7; 8; 11; 12; 13; 14 | |
| [2] $P42m$ (111) | 1; 2; 5; 6; 11; 12; 15; 16 | |
| [2] $P4mm$ (99) | 1; 2; 3; 4; 13; 14; 15; 16 | |
| [2] $P422$ (89) | 1; 2; 3; 4; 5; 6; 7; 8 | |
| [2] $P4/m11$ (83, $P4/m$) | 1; 2; 3; 4; 9; 10; 11; 12 | |
| [2] $P2/m12/m$ (65, $Cmmm$) | 1; 2; 7; 8; 9; 10; 15; 16 | $a - b, a + b, c$ |
| [2] $P2/m2/m1$ (47, $Pmmm$) | 1; 2; 5; 6; 9; 10; 13; 14 | |

II Maximal klassengleiche subgroups

● Enlarged unit cell

| | | | |
|---------------------------------|--|--------------------|---------------|
| [2] $c' = 2c$ | | | |
| $P4_2/mcm$ (132) | $\langle 2; 9; (3; 5) + (0, 0, 1) \rangle$ | $a, b, 2c$ | |
| $P4_2/mcm$ (132) | $\langle 2; 5; (3; 9) + (0, 0, 1) \rangle$ | $a, b, 2c$ | 0, 0, 1/2 |
| $P4_2/mmc$ (131) | $\langle 2; 5; 9; 3 + (0, 0, 1) \rangle$ | $a, b, 2c$ | |
| $P4_2/mmc$ (131) | $\langle 2; (3; 5; 9) + (0, 0, 1) \rangle$ | $a, b, 2c$ | 0, 0, 1/2 |
| $P4/mcc$ (124) | $\langle 2; 3; 9; 5 + (0, 0, 1) \rangle$ | $a, b, 2c$ | |
| $P4/mcc$ (124) | $\langle 2; 3; 5; 9 + (0, 0, 1) \rangle$ | $a, b, 2c$ | 0, 0, 1/2 |
| $P4/mmm$ (123) | $\langle 2; 3; 5; 9 \rangle$ | $a, b, 2c$ | |
| $P4/mmm$ (123) | $\langle 2; 3; (5; 9) + (0, 0, 1) \rangle$ | $a, b, 2c$ | 0, 0, 1/2 |
| [2] $a' = 2a, b' = 2b$ | | | |
| $C4/emc$ (129, $P4/nmm$) | $\langle 2; 3; (5; 9) + (1, 0, 0) \rangle$ | $a - b, a + b, c$ | 1/2, 0, 0 |
| $C4/emc$ (129, $P4/nmm$) | $\langle 2; 5; (3; 9) + (1, 0, 0) \rangle$ | $a - b, a + b, c$ | 0, 1/2, 0 |
| $C4/mmd$ (127, $P4/mbm$) | $\langle 2; 3; 9; 5 + (1, 0, 0) \rangle$ | $a - b, a + b, c$ | |
| $C4/mmd$ (127, $P4/mbm$) | $\langle 2; 5; 9; 3 + (1, 0, 0) \rangle$ | $a - b, a + b, c$ | 1/2, 1/2, 0 |
| $C4/emd$ (125, $P4/nbm$) | $\langle 2; 3; 5; 9 + (1, 0, 0) \rangle$ | $a - b, a + b, c$ | 1/2, 0, 0 |
| $C4/emd$ (125, $P4/nbm$) | $\langle 2; (3; 5) + (1, 0, 0); 9 + (0, 1, 0) \rangle$ | $a - b, a + b, c$ | 0, 1/2, 0 |
| $C4/mmm$ (123, $P4/mmm$) | $\langle 2; 3; 5; 9 \rangle$ | $a - b, a + b, c$ | |
| $C4/mmm$ (123, $P4/mmm$) | $\langle (2; 9) + (1, 1, 0); (3; 5) + (1, 0, 0) \rangle$ | $a - b, a + b, c$ | 1/2, 1/2, 0 |
| [2] $a' = 2a, b' = 2b, c' = 2c$ | | | |
| $F4/mmc$ (140, $I4/mcm$) | $\langle 2; 3; 9; 5 + (0, 0, 1) \rangle$ | $a - b, a + b, 2c$ | |
| $F4/mmc$ (140, $I4/mcm$) | $\langle 2; 3; 5; 9 + (0, 0, 1) \rangle$ | $a - b, a + b, 2c$ | 0, 0, 1/2 |
| $F4/mmc$ (140, $I4/mcm$) | $\langle 2; 5; 9; 3 + (0, 0, 1) \rangle$ | $a - b, a + b, 2c$ | 1/2, 1/2, 0 |
| $F4/mmc$ (140, $I4/mcm$) | $\langle 2; (3; 5; 9) + (0, 0, 1) \rangle$ | $a - b, a + b, 2c$ | 1/2, 1/2, 1/2 |
| $F4/mmm$ (139, $I4/mmm$) | $\langle 2; 3; 5; 9 \rangle$ | $a - b, a + b, 2c$ | |
| $F4/mmm$ (139, $I4/mmm$) | $\langle 2; 3; (5; 9) + (0, 0, 1) \rangle$ | $a - b, a + b, 2c$ | 0, 0, 1/2 |
| $F4/mmm$ (139, $I4/mmm$) | $\langle 2; 9; (3; 5) + (0, 0, 1) \rangle$ | $a - b, a + b, 2c$ | 1/2, 1/2, 0 |
| $F4/mmm$ (139, $I4/mmm$) | $\langle 2; 5; (3; 9) + (0, 0, 1) \rangle$ | $a - b, a + b, 2c$ | 1/2, 1/2, 1/2 |
| [3] $c' = 3c$ | | | |
| $P4/mmm$ (123) | $\langle 2; 3; 5; 9 \rangle$ | $a, b, 3c$ | |
| $P4/mmm$ (123) | $\langle 2; 3; (5; 9) + (0, 0, 2) \rangle$ | $a, b, 3c$ | 0, 0, 1 |
| $P4/mmm$ (123) | $\langle 2; 3; (5; 9) + (0, 0, 4) \rangle$ | $a, b, 3c$ | 0, 0, 2 |

● Series of maximal isomorphic subgroups

| | | | |
|------------------------------|--|-------------|-----------|
| [p] $c' = pc$ | | | |
| $P4/mmm$ (123) | $\langle 2; 3; (5; 9) + (0, 0, 2u) \rangle$ prime $p > 2$; $0 \leq u < p$ p conjugate subgroups | a, b, pc | 0, 0, u |
| [p^2] $a' = pa, b' = pb$ | | | |
| $P4/mmm$ (123) | $\langle (2; 9) + (2u, 2v, 0); 3 + (u + v, -u + v, 0); 5 + (2u, 0, 0) \rangle$ prime $p > 2$; $0 \leq u < p$; $0 \leq v < p$ p^2 conjugate subgroups | pa, pb, c | $u, v, 0$ |

I Minimal *translationengleiche* supergroups[3] $Pm\bar{3}m$ (221)**II Minimal non-isomorphic *klassengleiche* supergroups**

- Additional centring translations

[2] $I4/mmm$ (139)

- Decreased unit cell

none