

$P4_2/mmc$ 

No. 131

 $P4_2/m2/m2/c$ 
 $D_{4h}^9$ 
**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 | $r$ | 1 | (1) $x, y, z$                   | (2) $\bar{x}, \bar{y}, z$ | (3) $\bar{y}, x, z + \frac{1}{2}$        | (4) $y, \bar{x}, z + \frac{1}{2}$             |
|    |     |   | (5) $\bar{x}, y, \bar{z}$       | (6) $x, \bar{y}, \bar{z}$ | (7) $y, x, \bar{z} + \frac{1}{2}$        | (8) $\bar{y}, \bar{x}, \bar{z} + \frac{1}{2}$ |
|    |     |   | (9) $\bar{x}, \bar{y}, \bar{z}$ | (10) $x, y, \bar{z}$      | (11) $y, \bar{x}, \bar{z} + \frac{1}{2}$ | (12) $\bar{y}, x, \bar{z} + \frac{1}{2}$      |
|    |     |   | (13) $x, \bar{y}, z$            | (14) $\bar{x}, y, z$      | (15) $\bar{y}, \bar{x}, z + \frac{1}{2}$ | (16) $y, x, z + \frac{1}{2}$                  |

**I Maximal translationengleiche subgroups**

|                                |                            |                            |           |
|--------------------------------|----------------------------|----------------------------|-----------|
| [2] $P4_2m2$ (115)             | 1; 2; 7; 8; 11; 12; 13; 14 |                            | 0, 0, 1/4 |
| [2] $P4_2c$ (112)              | 1; 2; 5; 6; 11; 12; 15; 16 |                            | 0, 0, 1/4 |
| [2] $P4_2mc$ (105)             | 1; 2; 3; 4; 13; 14; 15; 16 |                            |           |
| [2] $P4_222$ (93)              | 1; 2; 3; 4; 5; 6; 7; 8     |                            |           |
| [2] $P4_2/m11$ (84, $P4_2/m$ ) | 1; 2; 3; 4; 9; 10; 11; 12  |                            |           |
| [2] $P2/m12/c$ (66, $Cccm$ )   | 1; 2; 7; 8; 9; 10; 15; 16  | $\mathbf{a - b, a + b, c}$ |           |
| [2] $P2/m2/m1$ (47, $Pmmm$ )   | 1; 2; 5; 6; 9; 10; 13; 14  |                            |           |

**II Maximal klassengleiche subgroups**

## • Enlarged unit cell

|  |  |                            |             |
|--|--|----------------------------|-------------|
| [2] $\mathbf{a}' = 2\mathbf{a}, \mathbf{b}' = 2\mathbf{b}$ |  |                            |             |
| $C4_2/emc$ (138, $P4_2/ncm$ )                              | $\langle 2; 3; (5; 9) + (1, 0, 0) \rangle$             | $\mathbf{a - b, a + b, c}$ | 1/2, 0, 0   |
| $C4_2/emc$ (138, $P4_2/ncm$ )                              | $\langle 2; 5; (3; 9) + (1, 0, 0) \rangle$             | $\mathbf{a - b, a + b, c}$ | 0, 1/2, 0   |
| $C4_2/mmd$ (136, $P4_2/mnm$ )                              | $\langle 2; 5; 9; 3 + (1, 0, 0) \rangle$               | $\mathbf{a - b, a + b, c}$ |             |
| $C4_2/mmd$ (136, $P4_2/mnm$ )                              | $\langle 2; 3; 9; 5 + (1, 0, 0) \rangle$               | $\mathbf{a - b, a + b, c}$ | 1/2, 1/2, 0 |
| $C4_2/emd$ (134, $P4_2/nm$ )                               | $\langle 2; 3; 5; 9 + (1, 0, 0) \rangle$               | $\mathbf{a - b, a + b, c}$ | 1/2, 0, 0   |
| $C4_2/emd$ (134, $P4_2/nm$ )                               | $\langle 2; (3; 5; 9) + (1, 0, 0) \rangle$             | $\mathbf{a - b, a + b, c}$ | 0, 1/2, 0   |
| $C4_2/mmc$ (132, $P4_2/mcm$ )                              | $\langle 2; 3; 5; 9 \rangle$                           | $\mathbf{a - b, a + b, c}$ |             |
| $C4_2/mmc$ (132, $P4_2/mcm$ )                              | $\langle 2; 9; (3; 5) + (1, 0, 0) \rangle$             | $\mathbf{a - b, a + b, c}$ | 1/2, 1/2, 0 |
| [3] $\mathbf{c}' = 3\mathbf{c}$                            |  |                            |             |
| $P4_2/mmc$ (131)   | $\langle 2; 5; 9; 3 + (0, 0, 1) \rangle$               | $\mathbf{a, b, 3c}$        |             |
| $P4_2/mmc$ (131)   | $\langle 2; 3 + (0, 0, 1); (5; 9) + (0, 0, 2) \rangle$ | $\mathbf{a, b, 3c}$        | 0, 0, 1     |
| $P4_2/mmc$ (131)   | $\langle 2; 3 + (0, 0, 1); (5; 9) + (0, 0, 4) \rangle$ | $\mathbf{a, b, 3c}$        | 0, 0, 2     |

## • Series of maximal isomorphic subgroups

|  |   |                      |           |
|--|---|----------------------|-----------|
| [ $p$ ] $\mathbf{c}' = p\mathbf{c}$                              |   |                      |           |
| $P4_2/mmc$ (131)   | $\langle 2; 3 + (0, 0, \frac{p}{2} - \frac{1}{2}); (5; 9) + (0, 0, 2u) \rangle$<br>$p > 2; 0 \leq u < p$              | $\mathbf{a, b, pc}$  | 0, 0, $u$ |
|  | $p$ conjugate subgroups for the prime $p$   |                      |           |
| [ $p^2$ ] $\mathbf{a}' = p\mathbf{a}, \mathbf{b}' = p\mathbf{b}$ |   |                      |           |
| $P4_2/mmc$ (131)   | $\langle (2; 9) + (2u, 2v, 0); 3 + (u + v, -u + v, 0); 5 + (2u, 0, 0) \rangle$<br>$p > 2; 0 \leq u < p; 0 \leq v < p$ | $\mathbf{pa, pb, c}$ | $u, v, 0$ |
|  | $p^2$ conjugate subgroups for the prime $p$   |                      |           |

**I Minimal translationengleiche supergroups**

 [3]  $Pm\bar{3}n$  (223)

**II Minimal non-isomorphic klassengleiche supergroups**

## • Additional centring translations

 [2]  $C4_2/mmc$  (132,  $P4_2/mcm$ ); [2]  $I4/mmm$  (139)

## • Decreased unit cell

 [2]  $\mathbf{c}' = \frac{1}{2}\mathbf{c}$   $P4/mmm$  (123)