

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

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] $P4n2$ (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	$\mathbf{a - b, a + b, c}$	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] $\mathbf{c}' = 3\mathbf{c}$			
$\left\{ \begin{array}{l} P4/mnc \text{ (128)} \\ P4/mnc \text{ (128)} \\ P4/mnc \text{ (128)} \end{array} \right.$	$\langle 2; 3; 9; 5 + (0, 0, 1) \rangle$	$\mathbf{a, b, 3c}$	
	$\langle 2; 3; 5 + (0, 0, 3); 9 + (0, 0, 2) \rangle$	$\mathbf{a, b, 3c}$	0, 0, 1
	$\langle 2; 3; 5 + (0, 0, 5); 9 + (0, 0, 4) \rangle$	$\mathbf{a, b, 3c}$	0, 0, 2

## • Series of maximal isomorphic subgroups

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

**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)