

$P4/nmm$ 

No. 129

 $P4/n2_1/m2/m$ 
 $D_{4h}^7$ 

 ORIGIN CHOICE 1, Origin at  $\bar{4}m2$  at  $\bar{4}/nm2/g$ , at  $-\frac{1}{4}, \frac{1}{4}, 0$  from centre ( $2/m$ )

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

**I Maximal translationengleiche subgroups**

[2] $P\bar{4}m2$ (115)	1; 2; 7; 8; 11; 12; 13; 14	
[2] $P\bar{4}2_1m$ (113)	1; 2; 5; 6; 11; 12; 15; 16	
[2] $P4mm$ (99)	1; 2; 3; 4; 13; 14; 15; 16	$1/2, 0, 0$
[2] $P42_12$ (90)	1; 2; 3; 4; 5; 6; 7; 8	
[2] $P4/n11$ (85, $P4/n$ )	1; 2; 3; 4; 9; 10; 11; 12	
[2] $P2/n12/m$ (67, $Cmme$ )	1; 2; 7; 8; 9; 10; 15; 16	$\mathbf{a} - \mathbf{b}, \mathbf{a} + \mathbf{b}, \mathbf{c}$
[2] $P2/n2_1/m1$ (59, $Pmnm$ )	1; 2; 5; 6; 9; 10; 13; 14	$1/4, 3/4, 0$

**II Maximal klassengleiche subgroups**

## • Enlarged unit cell

[2] $\mathbf{c}' = 2\mathbf{c}$		
$P4_2/ncm$ (138)	$\langle 2; 9; (3; 5) + (0, 0, 1) \rangle$	$\mathbf{a}, \mathbf{b}, 2\mathbf{c}$
$P4_2/ncm$ (138)	$\langle 2; 5; (3; 9) + (0, 0, 1) \rangle$	$\mathbf{a}, \mathbf{b}, 2\mathbf{c}$
$P4_2/nmc$ (137)	$\langle 2; 5; 9; 3 + (0, 0, 1) \rangle$	$\mathbf{a}, \mathbf{b}, 2\mathbf{c}$
$P4_2/nmc$ (137)	$\langle 2; (3; 5; 9) + (0, 0, 1) \rangle$	$\mathbf{a}, \mathbf{b}, 2\mathbf{c}$
$P4/ncc$ (130)	$\langle 2; 3; 9; 5 + (0, 0, 1) \rangle$	$\mathbf{a}, \mathbf{b}, 2\mathbf{c}$
$P4/ncc$ (130)	$\langle 2; 3; 5; 9 + (0, 0, 1) \rangle$	$\mathbf{a}, \mathbf{b}, 2\mathbf{c}$
$P4/nmm$ (129)	$\langle 2; 3; 5; 9 \rangle$	$\mathbf{a}, \mathbf{b}, 2\mathbf{c}$
$P4/nmm$ (129)	$\langle 2; 3; (5; 9) + (0, 0, 1) \rangle$	$\mathbf{a}, \mathbf{b}, 2\mathbf{c}$
[3] $\mathbf{c}' = 3\mathbf{c}$		
$P4/nmm$ (129)	$\langle 2; 3; 5; 9 \rangle$	$\mathbf{a}, \mathbf{b}, 3\mathbf{c}$
$P4/nmm$ (129)	$\langle 2; 3; (5; 9) + (0, 0, 2) \rangle$	$\mathbf{a}, \mathbf{b}, 3\mathbf{c}$
$P4/nmm$ (129)	$\langle 2; 3; (5; 9) + (0, 0, 4) \rangle$	$\mathbf{a}, \mathbf{b}, 3\mathbf{c}$

## • Series of maximal isomorphic subgroups

[ <i>p</i> ] $\mathbf{c}' = p\mathbf{c}$		
$P4/nmm$ (129)	$\langle 2; 3; (5; 9) + (0, 0, 2u) \rangle$ prime $p > 2$ ; $0 \leq u < p$ $p$ conjugate subgroups	$\mathbf{a}, \mathbf{b}, p\mathbf{c}$
[ $p^2$ ] $\mathbf{a}' = p\mathbf{a}, \mathbf{b}' = p\mathbf{b}$		
$P4/nmm$ (129)	$\langle 2 + (2u, 2v, 0); 3 + (\frac{p}{2} - \frac{1}{2} + u + v, \frac{p}{2} - \frac{1}{2} - u + v, 0); 5 + (\frac{p}{2} - \frac{1}{2} + 2u, \frac{p}{2} - \frac{1}{2}, 0); 9 + (\frac{p}{2} - \frac{1}{2} + 2u, \frac{p}{2} - \frac{1}{2} + 2v, 0) \rangle$ prime $p > 2$ ; $0 \leq u < p$ ; $0 \leq v < p$ $p^2$ conjugate subgroups	$p\mathbf{a}, p\mathbf{b}, \mathbf{c}$

**I Minimal translationengleiche supergroups**

none

**II Minimal non-isomorphic klassengleiche supergroups**

## • Additional centring translations

 [2]  $C4/mmm$  (123,  $P4/mmm$ ); [2]  $I4/mmm$  (139)

## • Decreased unit cell

none

ORIGIN CHOICE 2, Origin at centre ( $2/m$ ) at  $n2_1(2/m, 2_1/g)$ , at  $\frac{1}{4}, -\frac{1}{4}, 0$  from  $\bar{4}m2$

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

I Maximal translationengleiche subgroups

[2] $P\bar{4}m2$ (115)	1; 2; 7; 8; 11; 12; 13; 14		1/4, 3/4, 0
[2] $P\bar{4}2_1m$ (113)	1; 2; 5; 6; 11; 12; 15; 16		1/4, 3/4, 0
[2] $P4mm$ (99)	1; 2; 3; 4; 13; 14; 15; 16		1/4, 1/4, 0
[2] $P42_12$ (90)	1; 2; 3; 4; 5; 6; 7; 8		1/4, 3/4, 0
[2] $P4/n11$ (85, $P4/n$ )	1; 2; 3; 4; 9; 10; 11; 12		
[2] $P2/n12/m$ (67, $Cmme$ )	1; 2; 7; 8; 9; 10; 15; 16	$a - b, a + b, c$	
[2] $P2/n2_1/m1$ (59, $Pmnm$ )	1; 2; 5; 6; 9; 10; 13; 14		

II Maximal klassengleiche subgroups

• Enlarged unit cell

[2] $c' = 2c$			
$P4_2/ncm$ (138)	$\langle 2; 9; (3; 5) + (0,0,1) \rangle$	$a, b, 2c$	
$P4_2/ncm$ (138)	$\langle 2; 5; (3; 9) + (0,0,1) \rangle$	$a, b, 2c$	0, 0, 1/2
$P4_2/nmc$ (137)	$\langle 2; 5; 9; 3 + (0,0,1) \rangle$	$a, b, 2c$	
$P4_2/nmc$ (137)	$\langle 2; (3; 5; 9) + (0,0,1) \rangle$	$a, b, 2c$	0, 0, 1/2
$P4/ncc$ (130)	$\langle 2; 3; 9; 5 + (0,0,1) \rangle$	$a, b, 2c$	
$P4/ncc$ (130)	$\langle 2; 3; 5; 9 + (0,0,1) \rangle$	$a, b, 2c$	0, 0, 1/2
$P4/nmm$ (129)	$\langle 2; 3; 5; 9 \rangle$	$a, b, 2c$	
$P4/nmm$ (129)	$\langle 2; 3; (5; 9) + (0,0,1) \rangle$	$a, b, 2c$	0, 0, 1/2
[3] $c' = 3c$			
$P4/nmm$ (129)	$\langle 2; 3; 5; 9 \rangle$	$a, b, 3c$	
$P4/nmm$ (129)	$\langle 2; 3; (5; 9) + (0,0,2) \rangle$	$a, b, 3c$	0, 0, 1
$P4/nmm$ (129)	$\langle 2; 3; (5; 9) + (0,0,4) \rangle$	$a, b, 3c$	0, 0, 2

• Series of maximal isomorphic subgroups

[p] $c' = pc$			
$P4/nmm$ (129)	$\langle 2; 3; (5; 9) + (0,0,2u) \rangle$ prime $p > 2$ ; $0 \leq u < p$ $p$ conjugate subgroups	$a, b, pc$	0, 0, $u$
[ $p^2$ ] $a' = pa, b' = pb$			
$P4/nmm$ (129)	$\langle 2 + (\frac{p}{2} - \frac{1}{2} + 2u, \frac{p}{2} - \frac{1}{2} + 2v, 0);$ $3 + (\frac{p}{2} - \frac{1}{2} + u + v, -u + v, 0); 5 + (2u, \frac{p}{2} - \frac{1}{2}, 0);$ $9 + (2u, 2v, 0) \rangle$ 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

none

II Minimal non-isomorphic klassengleiche supergroups

• Additional centring translations

[2]  $C4/mmm$  (123,  $P4/mmm$ ); [2]  $I4/mmm$  (139)

• Decreased unit cell

none