

$P4/nbm$

No. 125

 $P4/n2/b2/m$
 D_{4h}^3

 ORIGIN CHOICE 1, Origin at 422 at $4/n22/g$, 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	n	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) $\bar{x} + \frac{1}{2}, \bar{y} + \frac{1}{2}, \bar{z}$	(10) $x + \frac{1}{2}, y + \frac{1}{2}, \bar{z}$	(11) $y + \frac{1}{2}, \bar{x} + \frac{1}{2}, \bar{z}$	(12) $\bar{y} + \frac{1}{2}, x + \frac{1}{2}, \bar{z}$
			(13) $x + \frac{1}{2}, \bar{y} + \frac{1}{2}, z$	(14) $\bar{x} + \frac{1}{2}, y + \frac{1}{2}, z$	(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] $P4b2$ (117)	1; 2; 7; 8; 11; 12; 13; 14		0, 1/2, 0
[2] $P42m$ (111)	1; 2; 5; 6; 11; 12; 15; 16		0, 1/2, 0
[2] $P4bm$ (100)	1; 2; 3; 4; 13; 14; 15; 16		
[2] $P422$ (89)	1; 2; 3; 4; 5; 6; 7; 8		
[2] $P4/n11$ (85, $P4/n$)	1; 2; 3; 4; 9; 10; 11; 12		0, 1/2, 0
[2] $P2/n12/m$ (67, $Cmme$)	1; 2; 7; 8; 9; 10; 15; 16	$\mathbf{a - b, a + b, c}$	1/4, 3/4, 0
[2] $P2/n2/b1$ (50, $Pban$)	1; 2; 5; 6; 9; 10; 13; 14		

II Maximal klassengleiche subgroups

• Enlarged unit cell

[2] $\mathbf{c}' = 2\mathbf{c}$			
$P4_2/nm$ (134)	$\langle 2; 9; (3; 5) + (0, 0, 1) \rangle$	$\mathbf{a, b, 2c}$	0, 1/2, 1/2
$P4_2/nm$ (134)	$\langle 2; 5; (3; 9) + (0, 0, 1) \rangle$	$\mathbf{a, b, 2c}$	0, 1/2, 0
$P4_2/nbc$ (133)	$\langle 2; 5; 9; 3 + (0, 0, 1) \rangle$	$\mathbf{a, b, 2c}$	0, 1/2, 1/2
$P4_2/nbc$ (133)	$\langle 2; (3; 5; 9) + (0, 0, 1) \rangle$	$\mathbf{a, b, 2c}$	0, 1/2, 0
$P4/nmc$ (126)	$\langle 2; 3; 9; 5 + (0, 0, 1) \rangle$	$\mathbf{a, b, 2c}$	0, 0, 1/2
$P4/nmc$ (126)	$\langle 2; 3; 5; 9 + (0, 0, 1) \rangle$	$\mathbf{a, b, 2c}$	
$P4/nbm$ (125)	$\langle 2; 3; 5; 9 \rangle$	$\mathbf{a, b, 2c}$	
$P4/nbm$ (125)	$\langle 2; 3; (5; 9) + (0, 0, 1) \rangle$	$\mathbf{a, b, 2c}$	0, 0, 1/2
[3] $\mathbf{c}' = 3\mathbf{c}$			
$P4/nbm$ (125)	$\langle 2; 3; 5; 9 \rangle$	$\mathbf{a, b, 3c}$	
$P4/nbm$ (125)	$\langle 2; 3; (5; 9) + (0, 0, 2) \rangle$	$\mathbf{a, b, 3c}$	0, 0, 1
$P4/nbm$ (125)	$\langle 2; 3; (5; 9) + (0, 0, 4) \rangle$	$\mathbf{a, b, 3c}$	0, 0, 2

• Series of maximal isomorphic subgroups

[p] $\mathbf{c}' = p\mathbf{c}$			
$P4/nbm$ (125)	$\langle 2; 3; (5; 9) + (0, 0, 2u) \rangle$ prime $p > 2$; $0 \leq u < p$ p conjugate subgroups	$\mathbf{a, b, pc}$	0, 0, u
[p^2] $\mathbf{a}' = p\mathbf{a}, \mathbf{b}' = p\mathbf{b}$			
$P4/nbm$ (125)	$\langle 2 + (2u, 2v, 0); 3 + (u + v, -u + v, 0); 5 + (2u, 0, 0); 9 + (\frac{p}{2} - \frac{1}{2} + 2u, \frac{p}{2} - \frac{1}{2} + 2v, 0) \rangle$ prime $p > 2$; $0 \leq u < p$; $0 \leq v < p$ p^2 conjugate subgroups	$\mathbf{pa, pb, c}$	$u, v, 0$

I Minimal translationengleiche supergroups

none

II Minimal non-isomorphic klassengleiche supergroups

• Additional centring translations

 [2] $C4/mmm$ (123, $P4/mmm$); [2] $I4/mcm$ (140)

• Decreased unit cell

none

ORIGIN CHOICE 2, Origin at centre ($2/m$) at $n(b,a)(2_1/g,2/m)$, at $\frac{1}{4}, \frac{1}{4}, 0$ from 422

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	n	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) $\bar{x} + \frac{1}{2}, y, \bar{z}$	(6) $x, \bar{y} + \frac{1}{2}, \bar{z}$	(7) y, x, \bar{z}	(8) $\bar{y} + \frac{1}{2}, \bar{x} + \frac{1}{2}, \bar{z}$
			(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) $x + \frac{1}{2}, \bar{y}, z$	(14) $\bar{x}, y + \frac{1}{2}, z$	(15) \bar{y}, \bar{x}, z	(16) $y + \frac{1}{2}, x + \frac{1}{2}, z$

I Maximal translationengleiche subgroups

[2] $P4b2$ (117)	1; 2; 7; 8; 11; 12; 13; 14		1/4, 3/4, 0
[2] $P4_2m$ (111)	1; 2; 5; 6; 11; 12; 15; 16		1/4, 3/4, 0
[2] $P4bm$ (100)	1; 2; 3; 4; 13; 14; 15; 16		1/4, 1/4, 0
[2] $P4_22$ (89)	1; 2; 3; 4; 5; 6; 7; 8		1/4, 1/4, 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	$a - b, a + b, c$	0, 1/2, 0
[2] $P2/n2/b1$ (50, $Pban$)	1; 2; 5; 6; 9; 10; 13; 14		

II Maximal klassengleiche subgroups

• Enlarged unit cell

[2] $c' = 2c$			
$P4_2/nm$ (134)	$\langle 2; 9; (3; 5) + (0,0,1) \rangle$	$a, b, 2c$	
$P4_2/nm$ (134)	$\langle 2; 5; (3; 9) + (0,0,1) \rangle$	$a, b, 2c$	0, 0, 1/2
$P4_2/nbc$ (133)	$\langle 2; 5; 9; 3 + (0,0,1) \rangle$	$a, b, 2c$	
$P4_2/nbc$ (133)	$\langle 2; (3; 5; 9) + (0,0,1) \rangle$	$a, b, 2c$	0, 0, 1/2
$P4/nnc$ (126)	$\langle 2; 3; 9; 5 + (0,0,1) \rangle$	$a, b, 2c$	
$P4/nnc$ (126)	$\langle 2; 3; 5; 9 + (0,0,1) \rangle$	$a, b, 2c$	0, 0, 1/2
$P4/nbm$ (125)	$\langle 2; 3; 5; 9 \rangle$	$a, b, 2c$	
$P4/nbm$ (125)	$\langle 2; 3; (5; 9) + (0,0,1) \rangle$	$a, b, 2c$	0, 0, 1/2
[3] $c' = 3c$			
$P4/nbm$ (125)	$\langle 2; 3; 5; 9 \rangle$	$a, b, 3c$	
$P4/nbm$ (125)	$\langle 2; 3; (5; 9) + (0,0,2) \rangle$	$a, b, 3c$	0, 0, 1
$P4/nbm$ (125)	$\langle 2; 3; (5; 9) + (0,0,4) \rangle$	$a, b, 3c$	0, 0, 2

• Series of maximal isomorphic subgroups

[p] $c' = pc$			
$P4/nbm$ (125)	$\langle 2; 3; (5; 9) + (0,0,2u) \rangle$ prime $p > 2$; $0 \leq u < p$ p conjugate subgroups	a, b, pc	0, 0, u
[p ²] $a' = pa, b' = pb$			
$P4/nbm$ (125)	$\langle 2 + (\frac{p}{2} - \frac{1}{2} + 2u, \frac{p}{2} - \frac{1}{2} + 2v, 0);$ $3 + (\frac{p}{2} - \frac{1}{2} + u + v, -u + v, 0); 5 + (\frac{p}{2} - \frac{1}{2} + 2u, 0, 0);$ $9 + (2u, 2v, 0) \rangle$ 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] $I4/mcm$ (140)

• Decreased unit cell

none