

$P4/nnc$

No. 126

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

 ORIGIN CHOICE 1, Origin at $422/n$, at $-\frac{1}{4}, -\frac{1}{4}, -\frac{1}{4}$ from $\bar{1}$

 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}, \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) $\bar{x} + \frac{1}{2}, \bar{y} + \frac{1}{2}, \bar{z} + \frac{1}{2}$	(10) $x + \frac{1}{2}, y + \frac{1}{2}, \bar{z} + \frac{1}{2}$	(11) $y + \frac{1}{2}, \bar{x} + \frac{1}{2}, \bar{z} + \frac{1}{2}$	(12) $\bar{y} + \frac{1}{2}, x + \frac{1}{2}, \bar{z} + \frac{1}{2}$
			(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		0, 1/2, 1/4
[2] $P42c$ (112)	1; 2; 5; 6; 11; 12; 15; 16		0, 1/2, 1/4
[2] $P4nc$ (104)	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, 1/4
[2] $P2/n12/c$ (68, $Ccce$)	1; 2; 7; 8; 9; 10; 15; 16	$\mathbf{a - b, a + b, c}$	
[2] $P2/n2/n1$ (48, $Pnmm$)	1; 2; 5; 6; 9; 10; 13; 14		

II Maximal klassengleiche subgroups

• Enlarged unit cell

[3] $\mathbf{c}' = 3\mathbf{c}$			
$\left\{ \begin{array}{l} P4/nmc \text{ (126)} \\ P4/nmc \text{ (126)} \\ P4/nmc \text{ (126)} \end{array} \right.$	$\langle 2; 3; 5; 9 + (0, 0, 1) \rangle$	$\mathbf{a, b, 3c}$	
	$\langle 2; 3; 5 + (0, 0, 2); 9 + (0, 0, 3) \rangle$	$\mathbf{a, b, 3c}$	0, 0, 1
	$\langle 2; 3; 5 + (0, 0, 4); 9 + (0, 0, 5) \rangle$	$\mathbf{a, b, 3c}$	0, 0, 2

• Series of maximal isomorphic subgroups

[p] $\mathbf{c}' = p\mathbf{c}$			
$P4/nmc$ (126)	$\langle 2; 3; 5 + (0, 0, 2u); 9 + (0, 0, \frac{p}{2} - \frac{1}{2} + 2u) \rangle$	$\mathbf{a, b, pc}$	0, 0, u
	$p > 2; 0 \leq u < p$		
	p conjugate subgroups for the prime p		
[p^2] $\mathbf{a}' = p\mathbf{a}, \mathbf{b}' = p\mathbf{b}$			
$P4/nmc$ (126)	$\langle 2 + (2u, 2v, 0); 3 + (u + v, -u + v, 0); 5 + (2u, 0, 0); 9 + (\frac{p}{2} - \frac{1}{2} + 2u, \frac{p}{2} - \frac{1}{2} + 2v, 0) \rangle$	$\mathbf{pa, pb, c}$	$u, v, 0$
	$p > 2; 0 \leq u < p; 0 \leq v < p$		
	p^2 conjugate subgroups for the prime p		

I Minimal translationengleiche supergroups

 [3] $Pn\bar{3}n$ (222)

II Minimal non-isomorphic klassengleiche supergroups

• Additional centring translations

 [2] $I4/mmm$ (139); [2] $C4/mcc$ (124, $P4/mcc$)

• Decreased unit cell

 [2] $\mathbf{c}' = \frac{1}{2}\mathbf{c}$ $P4/nbm$ (125)

ORIGIN CHOICE 2, Origin at $\bar{1}$ at $nn(n, c)$, at $\frac{1}{4}, \frac{1}{4}, \frac{1}{4}$ 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	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) $\bar{x} + \frac{1}{2}, y, \bar{z} + \frac{1}{2}$	(6) $x, \bar{y} + \frac{1}{2}, \bar{z} + \frac{1}{2}$	(7) $y, x, \bar{z} + \frac{1}{2}$	(8) $\bar{y} + \frac{1}{2}, \bar{x} + \frac{1}{2}, \bar{z} + \frac{1}{2}$
			(9) $\bar{x}, \bar{y}, \bar{z}$	(10) $x + \frac{1}{2}, y + \frac{1}{2}, \bar{z}$	(11) $y + \frac{1}{2}, \bar{x}, \bar{z}$	(12) $\bar{y}, x + \frac{1}{2}, \bar{z}$
			(13) $x + \frac{1}{2}, \bar{y}, z + \frac{1}{2}$	(14) $\bar{x}, y + \frac{1}{2}, z + \frac{1}{2}$	(15) $\bar{y}, \bar{x}, z + \frac{1}{2}$	(16) $y + \frac{1}{2}, x + \frac{1}{2}, z + \frac{1}{2}$

I Maximal translationengleiche subgroups

[2] $P\bar{4}n2$ (118)	1; 2; 7; 8; 11; 12; 13; 14		1/4, 3/4, 0
[2] $P42c$ (112)	1; 2; 5; 6; 11; 12; 15; 16		1/4, 3/4, 0
[2] $P4nc$ (104)	1; 2; 3; 4; 13; 14; 15; 16		1/4, 1/4, 0
[2] $P422$ (89)	1; 2; 3; 4; 5; 6; 7; 8		1/4, 1/4, 1/4
[2] $P4/n11$ (85, $P4/n$)	1; 2; 3; 4; 9; 10; 11; 12		
[2] $P2/n12/c$ (68, $Ccce$)	1; 2; 7; 8; 9; 10; 15; 16	$\mathbf{a - b, a + b, c}$	
[2] $P2/n2/n1$ (48, $Pnnn$)	1; 2; 5; 6; 9; 10; 13; 14		

II Maximal klassengleiche subgroups

• Enlarged unit cell

[3] $\mathbf{c}' = 3\mathbf{c}$			
$\left\{ \begin{array}{l} P4/nnc \text{ (126)} \\ P4/nnc \text{ (126)} \\ P4/nnc \text{ (126)} \end{array} \right.$	$\langle 2; 3; 9; 5 + (0, 0, 1) \rangle$	$\mathbf{a, b, 3c}$	
	$\langle 2; 3; 5 + (0, 0, 3); 9 + (0, 0, 2) \rangle$	$\mathbf{a, b, 3c}$	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] $\mathbf{c}' = p\mathbf{c}$			
$P4/nnc$ (126)	$\langle 2; 3; 5 + (0, 0, \frac{p}{2} - \frac{1}{2} + 2u); 9 + (0, 0, 2u) \rangle$	$\mathbf{a, b, pc}$	0, 0, u
	$p > 2; 0 \leq u < p$		
	p conjugate subgroups for the prime p		
[p^2] $\mathbf{a}' = p\mathbf{a}, \mathbf{b}' = p\mathbf{b}$			
$P4/nnc$ (126)	$\langle 2 + (\frac{p}{2} - \frac{1}{2} + 2u, \frac{p}{2} - \frac{1}{2} - 2v, 0);$	$p\mathbf{a}, p\mathbf{b}, \mathbf{c}$	$u, v, 0$
	$3 + (\frac{p}{2} - \frac{1}{2} + u + v, -u + v, 0); 5 + (\frac{p}{2} - \frac{1}{2} + 2u, 0, 0);$		
	$9 + (2u, 2v, 0) \rangle$		
	$p > 2; 0 \leq u < p; 0 \leq v < p$		
	p^2 conjugate subgroups for the prime p		

I Minimal translationengleiche supergroups

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