

$P4/n$

No. 85

 $P4/n$
 C_{4h}^3

 ORIGIN CHOICE 1, Origin at $\bar{4}$ on n , at $-\frac{1}{4}, \frac{1}{4}, 0$ from $\bar{1}$

 Generators selected (1); $t(1,0,0)$; $t(0,1,0)$; $t(0,0,1)$; (2); (3); (5)

General position

 Multiplicity,
Wyckoff letter,
Site symmetry

Coordinates

8	g	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) $\bar{x} + \frac{1}{2}, \bar{y} + \frac{1}{2}, \bar{z}$	(6) $x + \frac{1}{2}, y + \frac{1}{2}, \bar{z}$	(7) y, \bar{x}, \bar{z}	(8) \bar{y}, x, \bar{z}

I Maximal translationengleiche subgroups

[2] $P\bar{4}$ (81)	1; 2; 7; 8		
[2] $P4$ (75)	1; 2; 3; 4		$1/2, 0, 0$
[2] $P2/n$ (13, $P112/a$)	1; 2; 5; 6	$-\mathbf{a} - \mathbf{b}, \mathbf{a}, \mathbf{c}$	$1/4, 1/4, 0$

II Maximal klassengleiche subgroups

• Enlarged unit cell

[2] $\mathbf{c}' = 2\mathbf{c}$			
$P4_2/n$ (86)	$\langle 2; 5; 3 + (0, 0, 1) \rangle$	$\mathbf{a}, \mathbf{b}, 2\mathbf{c}$	$0, 0, 1/2$
$P4_2/n$ (86)	$\langle 2; (3; 5) + (0, 0, 1) \rangle$	$\mathbf{a}, \mathbf{b}, 2\mathbf{c}$	
$P4/n$ (85)	$\langle 2; 3; 5 \rangle$	$\mathbf{a}, \mathbf{b}, 2\mathbf{c}$	
$P4/n$ (85)	$\langle 2; 3; 5 + (0, 0, 1) \rangle$	$\mathbf{a}, \mathbf{b}, 2\mathbf{c}$	$0, 0, 1/2$
[3] $\mathbf{c}' = 3\mathbf{c}$			
$P4/n$ (85)	$\langle 2; 3; 5 \rangle$	$\mathbf{a}, \mathbf{b}, 3\mathbf{c}$	
$P4/n$ (85)	$\langle 2; 3; 5 + (0, 0, 2) \rangle$	$\mathbf{a}, \mathbf{b}, 3\mathbf{c}$	$0, 0, 1$
$P4/n$ (85)	$\langle 2; 3; 5 + (0, 0, 4) \rangle$	$\mathbf{a}, \mathbf{b}, 3\mathbf{c}$	$0, 0, 2$

• Series of maximal isomorphic subgroups

[p] $\mathbf{c}' = p\mathbf{c}$			
$P4/n$ (85)	$\langle 2; 3; 5 + (0, 0, 2u) \rangle$ $p > 2; 0 \leq u < p$ p conjugate subgroups for the prime p	$\mathbf{a}, \mathbf{b}, p\mathbf{c}$	$0, 0, u$
[p^2] $\mathbf{a}' = p\mathbf{a}, \mathbf{b}' = p\mathbf{b}$			
$P4/n$ (85)	$\langle 2 + (2u, 2v, 0); 3 + (\frac{p}{2} - \frac{1}{2} + u + v, \frac{p}{2} - \frac{1}{2} - u + v, 0); 5 + (\frac{p}{2} - \frac{1}{2} + 2u, \frac{p}{2} - \frac{1}{2} + 2v, 0) \rangle$ $p > 2; 0 \leq u < p; 0 \leq v < p$ p^2 conjugate subgroups for prime $p \equiv 3 \pmod{4}$	$p\mathbf{a}, p\mathbf{b}, \mathbf{c}$	$u, v, 0$
[$p = q^2 + r^2$] $\mathbf{a}' = q\mathbf{a} - r\mathbf{b}, \mathbf{b}' = r\mathbf{a} + q\mathbf{b}$			
$P4/n$ (85)	$\langle 2 + (2u, 0, 0); 3 + (\frac{q}{2} + \frac{r}{2} - \frac{1}{2} + u, \frac{q}{2} - \frac{r}{2} - \frac{1}{2} - u, 0); 5 + (\frac{q}{2} + \frac{r}{2} - \frac{1}{2} + 2u, \frac{q}{2} - \frac{r}{2} - \frac{1}{2}, 0) \rangle$ $q > 0; r > 0; p > 4; 0 \leq u < p$ p conjugate subgroups for prime $p \equiv 1 \pmod{4}$	$q\mathbf{a} - r\mathbf{b}, r\mathbf{a} + q\mathbf{b}, \mathbf{c}$	$u, 0, 0$

I Minimal translationengleiche supergroups

 [2] $P4/nbm$ (125); [2] $P4/nnc$ (126); [2] $P4/nmm$ (129); [2] $P4/ncc$ (130)

II Minimal non-isomorphic klassengleiche supergroups

• Additional centring translations

 [2] $C4/m$ (83, $P4/m$); [2] $I4/m$ (87)

• Decreased unit cell

none

ORIGIN CHOICE 2, Origin at $\bar{1}$ on n , at $\frac{1}{4}, -\frac{1}{4}, 0$ from $\bar{4}$

Generators selected (1); $t(1,0,0)$; $t(0,1,0)$; $t(0,0,1)$; (2); (3); (5)

General position

Multiplicity,
Wyckoff letter,
Site symmetry

Coordinates

8	g	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) $\bar{x}, \bar{y}, \bar{z}$	(6) $x + \frac{1}{2}, y + \frac{1}{2}, \bar{z}$	(7) $y + \frac{1}{2}, \bar{x}, \bar{z}$	(8) $\bar{y}, x + \frac{1}{2}, \bar{z}$

I Maximal translationengleiche subgroups

[2] $P\bar{4}$ (81)	1; 2; 7; 8		1/4, 3/4, 0
[2] $P4$ (75)	1; 2; 3; 4		1/4, 1/4, 0
[2] $P2/n$ (13, $P112/a$)	1; 2; 5; 6	–a – b, a, c	0, 1/2, 0

II Maximal klassengleiche subgroups

• Enlarged unit cell

[2] $\mathbf{c}' = 2\mathbf{c}$			
$P4_2/n$ (86)	$\langle 2; 5; 3 + (0,0,1) \rangle$	a, b, 2c	0, 1/2, 0
$P4_2/n$ (86)	$\langle 2; (3; 5) + (0,0,1) \rangle$	a, b, 2c	0, 1/2, 1/2
$P4/n$ (85)	$\langle 2; 3; 5 \rangle$	a, b, 2c	
$P4/n$ (85)	$\langle 2; 3; 5 + (0,0,1) \rangle$	a, b, 2c	0, 0, 1/2
[3] $\mathbf{c}' = 3\mathbf{c}$			
$P4/n$ (85)	$\langle 2; 3; 5 \rangle$	a, b, 3c	
$P4/n$ (85)	$\langle 2; 3; 5 + (0,0,2) \rangle$	a, b, 3c	0, 0, 1
$P4/n$ (85)	$\langle 2; 3; 5 + (0,0,4) \rangle$	a, b, 3c	0, 0, 2

• Series of maximal isomorphic subgroups

[p] $\mathbf{c}' = p\mathbf{c}$			
$P4/n$ (85)	$\langle 2; 3; 5 + (0,0,2u) \rangle$ $p > 2; 0 \leq u < p$ p conjugate subgroups for the prime p	a, b, $p\mathbf{c}$	0, 0, u
[p^2] $\mathbf{a}' = p\mathbf{a}, \mathbf{b}' = p\mathbf{b}$			
$P4/n$ (85)	$\langle 2 + (\frac{p}{2} - \frac{1}{2} + 2u, \frac{p}{2} - \frac{1}{2} + 2v, 0);$ $3 + (\frac{p}{2} - \frac{1}{2} + u + v, -u + v, 0); 5 + (2u, 2v, 0) \rangle$ $p > 2; 0 \leq u < p; 0 \leq v < p$ p^2 conjugate subgroups for prime $p \equiv 3 \pmod{4}$	$p\mathbf{a}, p\mathbf{b}, \mathbf{c}$	$u, v, 0$
[$p = q^2 + r^2$] $\mathbf{a}' = q\mathbf{a} - r\mathbf{b}, \mathbf{b}' = r\mathbf{a} + q\mathbf{b}$			
$P4/n$ (85)	$\langle 2 + (\frac{q}{2} + \frac{r}{2} - \frac{1}{2} + 2u, \frac{q}{2} - \frac{r}{2} - \frac{1}{2}, 0);$ $3 + (\frac{q}{2} - \frac{1}{2} + u, -\frac{r}{2} - u, 0); 5 + (2u, 0, 0) \rangle$ $q > 0; q$ odd; $r > 1; r$ even; $p > 4; 0 \leq u < p$ p conjugate subgroups for each pair of q and r	$q\mathbf{a} - r\mathbf{b}, r\mathbf{a} + q\mathbf{b}, \mathbf{c}$	$u, 0, 0$
$P4/n$ (85)	$\langle 2 + (\frac{q}{2} + \frac{r}{2} + \frac{1}{2} + 2u, \frac{q}{2} - \frac{r}{2} - \frac{1}{2}, 0);$ $3 + (\frac{q}{2} + u, -\frac{r}{2} - \frac{1}{2} - u, 0); 5 + (1 + 2u, 0, 0) \rangle$ $q > 1; q$ even; $r > 0; r$ odd; $p > 4; 0 \leq u < p$ p conjugate subgroups for each pair of q and r	$q\mathbf{a} - r\mathbf{b}, r\mathbf{a} + q\mathbf{b}, \mathbf{c}$	$1/2 + u, 0, 0$

I Minimal translationengleiche supergroups

[2] $P4/nbm$ (125); [2] $P4/nnc$ (126); [2] $P4/nmm$ (129); [2] $P4/ncc$ (130)

II Minimal non-isomorphic klassengleiche supergroups

• Additional centring translations

[2] $C4/m$ (83, $P4/m$); [2] $I4/m$ (87)

• Decreased unit cell

none