

$P4/ncc$ 

No. 130

 $P4/n2_1/c2/c$ 
 $D_{4h}^8$ 

 ORIGIN CHOICE 1, Origin at  $\bar{4}/nccn$ , 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); (9)

**General position**

 Multiplicity,  
Wyckoff letter,  
Site symmetry

**Coordinates**

16	<i>g</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) $\bar{x} + \frac{1}{2}, y + \frac{1}{2}, \bar{z} + \frac{1}{2}$	(6) $x + \frac{1}{2}, \bar{y} + \frac{1}{2}, \bar{z} + \frac{1}{2}$	(7) $y, x, \bar{z} + \frac{1}{2}$	(8) $\bar{y}, \bar{x}, \bar{z} + \frac{1}{2}$
			(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) $x, \bar{y}, z + \frac{1}{2}$	(14) $\bar{x}, y, z + \frac{1}{2}$	(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] $P\bar{4}c2$ (116)	1; 2; 7; 8; 11; 12; 13; 14	
[2] $P\bar{4}_2c$ (114)	1; 2; 5; 6; 11; 12; 15; 16	
[2] $P4cc$ (103)	1; 2; 3; 4; 13; 14; 15; 16	0, 1/2, 0
[2] $P4_22$ (90)	1; 2; 3; 4; 5; 6; 7; 8	0, 0, 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	<b>a – b, a + b, c</b>
[2] $P2/n2_1/c1$ (56, $Pccn$ )	1; 2; 5; 6; 9; 10; 13; 14	0, 0, 1/4 1/4, 1/4, 0

**II Maximal klassengleiche subgroups**

## • Enlarged unit cell

[3] $\mathbf{c}' = 3\mathbf{c}$		
$P4/ncc$ (130)	$\langle 2; 3; 9; 5 + (0, 0, 1) \rangle$	<b>a, b, 3c</b>
$P4/ncc$ (130)	$\langle 2; 3; 5 + (0, 0, 3); 9 + (0, 0, 2) \rangle$	<b>a, b, 3c</b>
$P4/ncc$ (130)	$\langle 2; 3; 5 + (0, 0, 5); 9 + (0, 0, 4) \rangle$	<b>a, b, 3c</b>

## • Series of maximal isomorphic subgroups

[ <i>p</i> ] $\mathbf{c}' = p\mathbf{c}$		
$P4/ncc$ (130)	$\langle 2; 3; 5 + (0, 0, \frac{p}{2} - \frac{1}{2} + 2u); 9 + (0, 0, 2u) \rangle$ $p > 2; 0 \leq u < p$ $p$ conjugate subgroups for the prime $p$	<b>a, b, pc</b>
[ $p^2$ ] $\mathbf{a}' = p\mathbf{a}, \mathbf{b}' = p\mathbf{b}$		
$P4/ncc$ (130)	$\langle 2 + (2u, 2v, 0); 3 + (\frac{p}{2} - \frac{1}{2} + u + v, \frac{p}{2} - \frac{1}{2} - u + v, 0); 5 + (\frac{p}{2} - \frac{1}{2} + 2u, \frac{p}{2} - \frac{1}{2}, 0); 9 + (\frac{p}{2} - \frac{1}{2} + 2u, \frac{p}{2} - \frac{1}{2} + 2v, 0) \rangle$ $p > 2; 0 \leq u < p; 0 \leq v < p$ $p^2$ conjugate subgroups for the prime $p$	<b>pa, pb, c</b>

**I Minimal translationengleiche supergroups**

none

**II Minimal non-isomorphic klassengleiche supergroups**

## • Additional centring translations

 [2]  $C4/mcc$  (124,  $P4/mcc$ ); [2]  $I4/mcm$  (140)

## • Decreased unit cell

 [2]  $\mathbf{c}' = \frac{1}{2}\mathbf{c}$   $P4/nmm$  (129)

ORIGIN CHOICE 2, Origin at  $\bar{1}$  at  $n1(c, n)$ , 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); (9)

### General position

Multiplicity,  
Wyckoff letter,  
Site symmetry

### Coordinates

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

### I Maximal translationengleiche subgroups

[2] $P\bar{4}c2$ (116)	1; 2; 7; 8; 11; 12; 13; 14		$1/4, 3/4, 0$
[2] $P\bar{4}2_1c$ (114)	1; 2; 5; 6; 11; 12; 15; 16		$1/4, 3/4, 0$
[2] $P4cc$ (103)	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		$1/4, 3/4, 1/4$
[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	$\mathbf{a - b, a + b, c}$	$0, 1/2, 0$
[2] $P2/n2_1/c1$ (56, $Pccn$ )	1; 2; 5; 6; 9; 10; 13; 14		

### II Maximal klassengleiche subgroups

#### • Enlarged unit cell

[3] $\mathbf{c}' = 3\mathbf{c}$			
$\left\{ \begin{array}{l} P4/ncc \text{ (130)} \\ P4/ncc \text{ (130)} \\ P4/ncc \text{ (130)} \end{array} \right.$	$\langle 2; 3; 9; 5 + (0, 0, 1) \rangle$	$\mathbf{a, b, 3c}$	
	$\langle 2; 3; 5 + (0, 0, 3); 9 + (0, 0, 2) \rangle$	$\mathbf{a, b, 3c}$	$0, 0, 1$
	$\langle 2; 3; 5 + (0, 0, 5); 9 + (0, 0, 4) \rangle$	$\mathbf{a, b, 3c}$	$0, 0, 2$

#### • Series of maximal isomorphic subgroups

[ $p$ ] $\mathbf{c}' = p\mathbf{c}$			
$P4/ncc$ (130)	$\langle 2; 3; 5 + (0, 0, \frac{p}{2} - \frac{1}{2} + 2u); 9 + (0, 0, 2u) \rangle$	$\mathbf{a, b, pc}$	$0, 0, u$
	$p > 2; 0 \leq u < p$		
	$p$ conjugate subgroups for the prime $p$		
[ $p^2$ ] $\mathbf{a}' = p\mathbf{a}, \mathbf{b}' = p\mathbf{b}$			
$P4/ncc$ (130)	$\langle 2 + (\frac{p}{2} - \frac{1}{2} + 2u, \frac{p}{2} - \frac{1}{2} + 2v, 0);$	$p\mathbf{a}, p\mathbf{b}, \mathbf{c}$	$u, v, 0$
	$3 + (\frac{p}{2} - \frac{1}{2} + u + v, -u + v, 0); 5 + (2u, \frac{p}{2} - \frac{1}{2}, 0);$		
	$9 + (2u, 2v, 0) \rangle$		
	$p > 2; 0 \leq u < p; 0 \leq v < p$		
	$p^2$ conjugate subgroups for the prime $p$		

### I Minimal translationengleiche supergroups

none

### II Minimal non-isomorphic klassengleiche supergroups

#### • Additional centring translations

[2]  $C4/mcc$  (124,  $P4/mcc$ ); [2]  $I4/mcm$  (140)

#### • Decreased unit cell

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