

$P4_2/nbc$ 

No. 133

 $P4_2/n2/b2/c$ 
 $D_{4h}^{11}$ 

 ORIGIN CHOICE 1, Origin at  $\bar{4}12_1/c$ , 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	<i>k</i>	1	(1) $x, y, z$	(2) $\bar{x}, \bar{y}, z$	(3) $\bar{y} + \frac{1}{2}, x + \frac{1}{2}, z + \frac{1}{2}$	(4) $y + \frac{1}{2}, \bar{x} + \frac{1}{2}, z + \frac{1}{2}$
			(5) $\bar{x}, y, \bar{z} + \frac{1}{2}$	(6) $x, \bar{y}, \bar{z} + \frac{1}{2}$	(7) $y + \frac{1}{2}, x + \frac{1}{2}, \bar{z}$	(8) $\bar{y} + \frac{1}{2}, \bar{x} + \frac{1}{2}, \bar{z}$
			(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) $y, \bar{x}, \bar{z}$	(12) $\bar{y}, x, \bar{z}$
			(13) $x + \frac{1}{2}, \bar{y} + \frac{1}{2}, z$	(14) $\bar{x} + \frac{1}{2}, y + \frac{1}{2}, z$	(15) $\bar{y}, \bar{x}, z + \frac{1}{2}$	(16) $y, x, z + \frac{1}{2}$

**I Maximal translationengleiche subgroups**

[2] $P\bar{4}b2$ (117)	1; 2; 7; 8; 11; 12; 13; 14	
[2] $P\bar{4}2c$ (112)	1; 2; 5; 6; 11; 12; 15; 16	
[2] $P4_2bc$ (106)	1; 2; 3; 4; 13; 14; 15; 16	0, 1/2, 0
[2] $P4_222$ (93)	1; 2; 3; 4; 5; 6; 7; 8	0, 1/2, 1/4
[2] $P4_2/n11$ (86, $P4_2/n$ )	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> 1/2, 0, 0
[2] $P2/n2/b1$ (50, $Pban$ )	1; 2; 5; 6; 9; 10; 13; 14	0, 0, 1/4

**II Maximal klassengleiche subgroups**

## • Enlarged unit cell

[3] $\mathbf{c}' = 3\mathbf{c}$			
$\left\{ \begin{array}{l} P4_2/nbc \text{ (133)} \\ P4_2/nbc \text{ (133)} \\ P4_2/nbc \text{ (133)} \end{array} \right.$	$\langle 2; (3; 5; 9) + (0, 0, 1) \rangle$	<b>a, b, 3c</b>	
	$\langle 2; 3 + (0, 0, 1); (5; 9) + (0, 0, 3) \rangle$	<b>a, b, 3c</b>	0, 0, 1
	$\langle 2; 3 + (0, 0, 1); (5; 9) + (0, 0, 5) \rangle$	<b>a, b, 3c</b>	0, 0, 2

## • Series of maximal isomorphic subgroups

[ <i>p</i> ] $\mathbf{c}' = p\mathbf{c}$			
$P4_2/nbc$ (133)	$\langle 2; 3 + (0, 0, \frac{p}{2} - \frac{1}{2}); (5; 9) + (0, 0, \frac{p}{2} - \frac{1}{2} + 2u) \rangle$	<b>a, b, pc</b>	0, 0, <i>u</i>
	$p > 2; 0 \leq u < p$		
	$p$ conjugate subgroups for the prime $p$		
[ $p^2$ ] $\mathbf{a}' = p\mathbf{a}, \mathbf{b}' = p\mathbf{b}$			
$P4_2/nbc$ (133)	$\langle 2 + (2u, 2v, 0); 3 + (\frac{p}{2} - \frac{1}{2} + u + v, \frac{p}{2} - \frac{1}{2} - u + v, 0);$	<b>pa, pb, c</b>	<i>u, v, 0</i>
	$5 + (2u, 0, 0); 9 + (\frac{p}{2} - \frac{1}{2} + 2u, \frac{p}{2} - \frac{1}{2} + 2v, 0) \rangle$		
	$p > 2; 0 \leq u < p; 0 \leq v < p$		
	$p^2$ conjugate subgroups for the prime $p$		

**I Minimal translationengleiche supergroups**

none

**II Minimal non-isomorphic klassengleiche supergroups**

## • Additional centring translations

 [2]  $C4_2/mmc$  (132,  $P4_2/mcm$ ); [2]  $I4/mcm$  (140)

## • Decreased unit cell

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

ORIGIN CHOICE 2, Origin at  $\bar{1}$  at  $n(b, a)(n, c)$ , at  $\frac{1}{4}, -\frac{1}{4}, \frac{1}{4}$  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	$k$	1	(1) $x, y, z$	(2) $\bar{x} + \frac{1}{2}, \bar{y} + \frac{1}{2}, z$	(3) $\bar{y} + \frac{1}{2}, x, z + \frac{1}{2}$	(4) $y, \bar{x} + \frac{1}{2}, z + \frac{1}{2}$
			(5) $\bar{x} + \frac{1}{2}, y, \bar{z}$	(6) $x, \bar{y} + \frac{1}{2}, \bar{z}$	(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) $y + \frac{1}{2}, \bar{x}, \bar{z} + \frac{1}{2}$	(12) $\bar{y}, x + \frac{1}{2}, \bar{z} + \frac{1}{2}$
			(13) $x + \frac{1}{2}, \bar{y}, z$	(14) $\bar{x}, y + \frac{1}{2}, z$	(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] $P\bar{4}b2$ (117)	1; 2; 7; 8; 11; 12; 13; 14		$1/4, 3/4, 1/4$
[2] $P\bar{4}2c$ (112)	1; 2; 5; 6; 11; 12; 15; 16		$1/4, 3/4, 1/4$
[2] $P4_2bc$ (106)	1; 2; 3; 4; 13; 14; 15; 16		$1/4, 1/4, 0$
[2] $P4_222$ (93)	1; 2; 3; 4; 5; 6; 7; 8		$1/4, 1/4, 0$
[2] $P4_2/n11$ (86, $P4_2/n$ )	1; 2; 3; 4; 9; 10; 11; 12		$0, 1/2, 0$
[2] $P2/n12/c$ (68, $Ccce$ )	1; 2; 7; 8; 9; 10; 15; 16	$\mathbf{a - b, a + b, c}$	
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II Maximal klassengleiche subgroups

• Enlarged unit cell

[3] $\mathbf{c}' = 3\mathbf{c}$			
$\left\{ \begin{array}{l} P4_2/nbc \text{ (133)} \\ P4_2/nbc \text{ (133)} \\ P4_2/nbc \text{ (133)} \end{array} \right.$	$\langle 2; 5; 9; 3 + (0, 0, 1) \rangle$	$\mathbf{a, b, 3c}$	
	$\langle 2; 3 + (0, 0, 1); (5; 9) + (0, 0, 2) \rangle$	$\mathbf{a, b, 3c}$	$0, 0, 1$
	$\langle 2; 3 + (0, 0, 1); (5; 9) + (0, 0, 4) \rangle$	$\mathbf{a, b, 3c}$	$0, 0, 2$

• Series of maximal isomorphic subgroups

[ $p$ ] $\mathbf{c}' = p\mathbf{c}$			
$P4_2/nbc$ (133)	$\langle 2; 3 + (0, 0, \frac{p}{2} - \frac{1}{2}); (5; 9) + (0, 0, 2u) \rangle$	$\mathbf{a, b, pc}$	$0, 0, u$
	$p > 2; 0 \leq u < p$		
	$p$ conjugate subgroups for the prime $p$		
[ $p^2$ ] $\mathbf{a}' = p\mathbf{a}, \mathbf{b}' = p\mathbf{b}$			
$P4_2/nbc$ (133)	$\langle 2 + (\frac{p}{2} - \frac{1}{2} + 2u, \frac{p}{2} - \frac{1}{2} + 2v, 0);$	$p\mathbf{a}, p\mathbf{b}, \mathbf{c}$	$u, v, 0$
	$3 + (\frac{p}{2} - \frac{1}{2} + u + v, -u + v, 0); 5 + (\frac{p}{2} - \frac{1}{2} + 2u, 0, 0);$		
	$9 + (2u, 2v, 0) \rangle$		
	$p > 2; 0 \leq u < p; 0 \leq v < p$		
	$p^2$ conjugate subgroups for the prime $p$		

I Minimal translationengleiche supergroups

none

II Minimal non-isomorphic klassengleiche supergroups

• Additional centring translations

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