

$P4_2/nmc$ 

No. 137

 $P4_2/n2_1/m2/c$  $D_{4h}^{15}$ ORIGIN CHOICE 1, Origin at  $\bar{4}m2/n$ , 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	$h$	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) $\bar{x} + \frac{1}{2}, y + \frac{1}{2}, \bar{z} + \frac{1}{2}$	(6) $x + \frac{1}{2}, \bar{y} + \frac{1}{2}, \bar{z} + \frac{1}{2}$	(7) $y, x, \bar{z}$	(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) $y, \bar{x}, \bar{z}$	(12) $\bar{y}, x, \bar{z}$
			(13) $x, \bar{y}, z$	(14) $\bar{x}, y, z$	(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] $P\bar{4}m2$ (115)	1; 2; 7; 8; 11; 12; 13; 14	
[2] $P\bar{4}2_1c$ (114)	1; 2; 5; 6; 11; 12; 15; 16	
[2] $P4_2mc$ (105)	1; 2; 3; 4; 13; 14; 15; 16	0, 1/2, 0
[2] $P4_22_12$ (94)	1; 2; 3; 4; 5; 6; 7; 8	
[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	$\mathbf{a} - \mathbf{b}, \mathbf{a} + \mathbf{b}, \mathbf{c}$
[2] $P2/n2_1/m1$ (59, $Pmmn$ )	1; 2; 5; 6; 9; 10; 13; 14	0, 0, 1/4

II Maximal *klassengleiche* subgroups

## • Enlarged unit cell

[3] $\mathbf{c}' = 3\mathbf{c}$			
$P4_2/nmc$ (137)	$\langle 2; (3; 5; 9) + (0, 0, 1) \rangle$	$\mathbf{a}, \mathbf{b}, 3\mathbf{c}$	
$P4_2/nmc$ (137)	$\langle 2; 3 + (0, 0, 1); (5; 9) + (0, 0, 3) \rangle$	$\mathbf{a}, \mathbf{b}, 3\mathbf{c}$	0, 0, 1
$P4_2/nmc$ (137)	$\langle 2; 3 + (0, 0, 1); (5; 9) + (0, 0, 5) \rangle$	$\mathbf{a}, \mathbf{b}, 3\mathbf{c}$	0, 0, 2

## • Series of maximal isomorphic subgroups

[ $p$ ] $\mathbf{c}' = p\mathbf{c}$			
$P4_2/nmc$ (137)	$\langle 2; 3 + (0, 0, \frac{p}{2} - \frac{1}{2}); (5; 9) + (0, 0, \frac{p}{2} - \frac{1}{2} + 2u) \rangle$ prime $p > 2$ ; $0 \leq u < p$ $p$ conjugate subgroups	$\mathbf{a}, \mathbf{b}, p\mathbf{c}$	0, 0, $u$
[ $p^2$ ] $\mathbf{a}' = p\mathbf{a}, \mathbf{b}' = p\mathbf{b}$			
$P4_2/nmc$ (137)	$\langle 2 + (2u, 2v, 0); 3 + (\frac{p}{2} - \frac{1}{2} + u + v, \frac{p}{2} - \frac{1}{2} - u + v, 0); 5 + (\frac{p}{2} - \frac{1}{2} + 2u, \frac{p}{2} - \frac{1}{2}, 0); 9 + (\frac{p}{2} - \frac{1}{2} + 2u, \frac{p}{2} - \frac{1}{2} + 2v, 0) \rangle$ prime $p > 2$ ; $0 \leq u < p$ ; $0 \leq v < p$ $p^2$ conjugate subgroups	$p\mathbf{a}, p\mathbf{b}, \mathbf{c}$	$u, v, 0$

I Minimal *translationengleiche* supergroups

none

II Minimal non-isomorphic *klassengleiche* supergroups

## • Additional centring translations

[2]  $C4_2/nmc$  (132,  $P4_2/mcm$ ); [2]  $I4/mmm$  (139)

## • Decreased unit cell

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

ORIGIN CHOICE 2, Origin at  $\bar{1}$  at  $n2_1(c, n)$ , at  $\frac{1}{4}, -\frac{1}{4}, \frac{1}{4}$  from  $\bar{4}m2$

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	$h$	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) $\bar{x}, y + \frac{1}{2}, \bar{z}$	(6) $x + \frac{1}{2}, \bar{y}, \bar{z}$	(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) $y + \frac{1}{2}, \bar{x}, \bar{z} + \frac{1}{2}$	(12) $\bar{y}, x + \frac{1}{2}, \bar{z} + \frac{1}{2}$
			(13) $x, \bar{y} + \frac{1}{2}, z$	(14) $\bar{x} + \frac{1}{2}, y, z$	(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] $P\bar{4}m2$ (115)	1; 2; 7; 8; 11; 12; 13; 14		$1/4, 3/4, 1/4$
[2] $P\bar{4}2_1c$ (114)	1; 2; 5; 6; 11; 12; 15; 16		$1/4, 3/4, 1/4$
[2] $P4_2mc$ (105)	1; 2; 3; 4; 13; 14; 15; 16		$1/4, 1/4, 0$
[2] $P4_22_12$ (94)	1; 2; 3; 4; 5; 6; 7; 8		$1/4, 3/4, 1/4$
[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	$\mathbf{a - b, a + b, c}$	$0, 1/2, 0$
[2] $P2/n2_1/m1$ (59, $Pmnn$ )	1; 2; 5; 6; 9; 10; 13; 14		

**II Maximal klassengleiche subgroups**

• Enlarged unit cell

[3] $\mathbf{c}' = 3\mathbf{c}$			
$\left\{ \begin{array}{l} P4_2/nmc \text{ (137)} \\ P4_2/nmc \text{ (137)} \\ P4_2/nmc \text{ (137)} \end{array} \right.$	$\langle 2; 5; 9; 3 + (0,0,1) \rangle$	$\mathbf{a, b, 3c}$	
	$\langle 2; 3 + (0,0,1); (5; 9) + (0,0,2) \rangle$	$\mathbf{a, b, 3c}$	$0, 0, 1$
	$\langle 2; 3 + (0,0,1); (5; 9) + (0,0,4) \rangle$	$\mathbf{a, b, 3c}$	$0, 0, 2$

• Series of maximal isomorphic subgroups

[ $p$ ] $\mathbf{c}' = p\mathbf{c}$			
$P4_2/nmc$ (137)	$\langle 2; 3 + (0,0, \frac{p}{2} - \frac{1}{2}); (5; 9) + (0,0, 2u) \rangle$	$\mathbf{a, b, pc}$	$0, 0, u$
	prime $p > 2$ ; $0 \leq u < p$		
	$p$ conjugate subgroups		
[ $p^2$ ] $\mathbf{a}' = p\mathbf{a}, \mathbf{b}' = p\mathbf{b}$			
$P4_2/nmc$ (137)	$\langle 2 + (\frac{p}{2} - \frac{1}{2} + 2u, \frac{p}{2} - \frac{1}{2} + 2v, 0);$	$\mathbf{pa, pb, c}$	$u, v, 0$
	$3 + (\frac{p}{2} - \frac{1}{2} + u + v, -u + v, 0); 5 + (2u, \frac{p}{2} - \frac{1}{2}, 0);$		
	$9 + (2u, 2v, 0) \rangle$		
	prime $p > 2$ ; $0 \leq u < p$ ; $0 \leq v < p$		
	$p^2$ conjugate subgroups		

**I Minimal translationengleiche supergroups**

none

**II Minimal non-isomorphic klassengleiche supergroups**

• Additional centring translations

[2]  $C4_2/mmc$  (132,  $P4_2/mcm$ ); [2]  $I4/mmm$  (139)

• Decreased unit cell

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