

$D_{2d}^1$ 
 $P\bar{4}2m$ 

No. 111

 $P\bar{4}2m$ 
**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	<i>o</i>	1								
			(1)	$x, y, z$	(2)	$\bar{x}, \bar{y}, z$	(3)	$y, \bar{x}, \bar{z}$	(4)	$\bar{y}, x, \bar{z}$
			(5)	$\bar{x}, y, \bar{z}$	(6)	$x, \bar{y}, \bar{z}$	(7)	$\bar{y}, \bar{x}, z$	(8)	$y, x, z$

**I Maximal translationengleiche subgroups**

[2] $P\bar{4}11$ (81, $P\bar{4}$ )	1; 2; 3; 4	
[2] $P21m$ (35, $Cmm2$ )	1; 2; 7; 8	$\mathbf{a} - \mathbf{b}, \mathbf{a} + \mathbf{b}, \mathbf{c}$
[2] $P221$ (16, $P222$ )	1; 2; 5; 6	

**II Maximal klassengleiche subgroups**

## • Enlarged unit cell

[2] $\mathbf{c}' = 2\mathbf{c}$		
$P\bar{4}2c$ (112)	$\langle 2; 3; 5 + (0, 0, 1) \rangle$	$\mathbf{a}, \mathbf{b}, 2\mathbf{c}$
$P\bar{4}2c$ (112)	$\langle 2; 5; 3 + (0, 0, 1) \rangle$	$\mathbf{a}, \mathbf{b}, 2\mathbf{c}$ 0, 0, 1/2
$P\bar{4}2m$ (111)	$\langle 2; 3; 5 \rangle$	$\mathbf{a}, \mathbf{b}, 2\mathbf{c}$
$P\bar{4}2m$ (111)	$\langle 2; (3; 5) + (0, 0, 1) \rangle$	$\mathbf{a}, \mathbf{b}, 2\mathbf{c}$ 0, 0, 1/2
[2] $\mathbf{a}' = 2\mathbf{a}, \mathbf{b}' = 2\mathbf{b}$		
$C\bar{4}2d$ (117, $P\bar{4}b2$ )	$\langle 2; 3; 5 + (1, 0, 0) \rangle$	$\mathbf{a} - \mathbf{b}, \mathbf{a} + \mathbf{b}, \mathbf{c}$
$C\bar{4}2d$ (117, $P\bar{4}b2$ )	$\langle 2; 5; 3 + (1, 0, 0) \rangle$	$\mathbf{a} - \mathbf{b}, \mathbf{a} + \mathbf{b}, \mathbf{c}$ 1/2, 1/2, 0
$C\bar{4}2m$ (115, $P\bar{4}m2$ )	$\langle 2; 3; 5 \rangle$	$\mathbf{a} - \mathbf{b}, \mathbf{a} + \mathbf{b}, \mathbf{c}$
$C\bar{4}2m$ (115, $P\bar{4}m2$ )	$\langle 2; (3; 5) + (1, 0, 0) \rangle$	$\mathbf{a} - \mathbf{b}, \mathbf{a} + \mathbf{b}, \mathbf{c}$ 1/2, 1/2, 0
[2] $\mathbf{a}' = 2\mathbf{a}, \mathbf{b}' = 2\mathbf{b}, \mathbf{c}' = 2\mathbf{c}$		
$F\bar{4}2c$ (120, $I\bar{4}c2$ )	$\langle 2; 3; 5 + (0, 0, 1) \rangle$	$\mathbf{a} - \mathbf{b}, \mathbf{a} + \mathbf{b}, 2\mathbf{c}$
$F\bar{4}2c$ (120, $I\bar{4}c2$ )	$\langle 2; 5; 3 + (0, 0, 1) \rangle$	$\mathbf{a} - \mathbf{b}, \mathbf{a} + \mathbf{b}, 2\mathbf{c}$ 0, 0, 1/2
$F\bar{4}2m$ (119, $I\bar{4}m2$ )	$\langle 2; 3; 5 \rangle$	$\mathbf{a} - \mathbf{b}, \mathbf{a} + \mathbf{b}, 2\mathbf{c}$
$F\bar{4}2m$ (119, $I\bar{4}m2$ )	$\langle 2; (3; 5) + (0, 0, 1) \rangle$	$\mathbf{a} - \mathbf{b}, \mathbf{a} + \mathbf{b}, 2\mathbf{c}$ 0, 0, 1/2
[3] $\mathbf{c}' = 3\mathbf{c}$		
$P\bar{4}2m$ (111)	$\langle 2; 3; 5 \rangle$	$\mathbf{a}, \mathbf{b}, 3\mathbf{c}$
$P\bar{4}2m$ (111)	$\langle 2; (3; 5) + (0, 0, 2) \rangle$	$\mathbf{a}, \mathbf{b}, 3\mathbf{c}$ 0, 0, 1
$P\bar{4}2m$ (111)	$\langle 2; (3; 5) + (0, 0, 4) \rangle$	$\mathbf{a}, \mathbf{b}, 3\mathbf{c}$ 0, 0, 2

## • Series of maximal isomorphic subgroups

[ $p$ ] $\mathbf{c}' = p\mathbf{c}$		
$P\bar{4}2m$ (111)	$\langle 2; (3; 5) + (0, 0, 2u) \rangle$	$\mathbf{a}, \mathbf{b}, p\mathbf{c}$ 0, 0, $u$
	$p > 2; 0 \leq u < p$	
	$p$ conjugate subgroups for the prime $p$	
[ $p^2$ ] $\mathbf{a}' = p\mathbf{a}, \mathbf{b}' = p\mathbf{b}$		
$P\bar{4}2m$ (111)	$\langle 2 + (2u, 2v, 0); 3 + (u - v, u + v, 0); 5 + (2u, 0, 0) \rangle$	$p\mathbf{a}, p\mathbf{b}, \mathbf{c}$ $u, v, 0$
	$p > 2; 0 \leq u < p; 0 \leq v < p$	
	$p^2$ conjugate subgroups for the prime $p$	

**I Minimal translationengleiche supergroups**

 [2]  $P4/mmm$  (123); [2]  $P4/nbm$  (125); [2]  $P4_2/mcm$  (132); [2]  $P4_2/nm$  (134); [3]  $P\bar{4}3m$  (215)

**II Minimal non-isomorphic klassengleiche supergroups**

## • Additional centring translations

 [2]  $C\bar{4}2m$  (115,  $P\bar{4}m2$ ); [2]  $I\bar{4}2m$  (121)

## • Decreased unit cell

none