

D_{4h}^1 $P4/m2/m2/m$

No. 123

 $P4/mmm$ 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	u	1	(1) x, y, z	(2) \bar{x}, \bar{y}, z	(3) \bar{y}, x, z	(4) y, \bar{x}, z
			(5) \bar{x}, y, \bar{z}	(6) x, \bar{y}, \bar{z}	(7) y, x, \bar{z}	(8) $\bar{y}, \bar{x}, \bar{z}$
			(9) $\bar{x}, \bar{y}, \bar{z}$	(10) x, y, \bar{z}	(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}, \bar{x}, z	(16) y, x, z

I Maximal translationengleiche subgroups

[2] $P\bar{4}m2$ (115)	1; 2; 7; 8; 11; 12; 13; 14	
[2] $P42m$ (111)	1; 2; 5; 6; 11; 12; 15; 16	
[2] $P4mm$ (99)	1; 2; 3; 4; 13; 14; 15; 16	
[2] $P422$ (89)	1; 2; 3; 4; 5; 6; 7; 8	
[2] $P4/m11$ (83, $P4/m$)	1; 2; 3; 4; 9; 10; 11; 12	
[2] $P2/m12/m$ (65, $Cmmm$)	1; 2; 7; 8; 9; 10; 15; 16	$\mathbf{a - b, a + b, c}$
[2] $P2/m2/m1$ (47, $Pmmm$)	1; 2; 5; 6; 9; 10; 13; 14	

II Maximal klassengleiche subgroups

• Enlarged unit cell

[2] $\mathbf{c}' = 2\mathbf{c}$			
$P4_2/mcm$ (132)	$\langle 2; 9; (3; 5) + (0, 0, 1) \rangle$	$\mathbf{a, b, 2c}$	
$P4_2/mcm$ (132)	$\langle 2; 5; (3; 9) + (0, 0, 1) \rangle$	$\mathbf{a, b, 2c}$	0, 0, 1/2
$P4_2/mmc$ (131)	$\langle 2; 5; 9; 3 + (0, 0, 1) \rangle$	$\mathbf{a, b, 2c}$	
$P4_2/mmc$ (131)	$\langle 2; (3; 5; 9) + (0, 0, 1) \rangle$	$\mathbf{a, b, 2c}$	0, 0, 1/2
$P4/mcc$ (124)	$\langle 2; 3; 9; 5 + (0, 0, 1) \rangle$	$\mathbf{a, b, 2c}$	
$P4/mcc$ (124)	$\langle 2; 3; 5; 9 + (0, 0, 1) \rangle$	$\mathbf{a, b, 2c}$	0, 0, 1/2
$P4/mmm$ (123)	$\langle 2; 3; 5; 9 \rangle$	$\mathbf{a, b, 2c}$	
$P4/mmm$ (123)	$\langle 2; 3; (5; 9) + (0, 0, 1) \rangle$	$\mathbf{a, b, 2c}$	0, 0, 1/2
[2] $\mathbf{a}' = 2\mathbf{a}, \mathbf{b}' = 2\mathbf{b}$			
$C4/emm$ (129, $P4/nmm$)	$\langle 2; 3; (5; 9) + (1, 0, 0) \rangle$	$\mathbf{a - b, a + b, c}$	1/2, 0, 0
$C4/emm$ (129, $P4/nmm$)	$\langle 2; 5; (3; 9) + (1, 0, 0) \rangle$	$\mathbf{a - b, a + b, c}$	0, 1/2, 0
$C4/mmd$ (127, $P4/mbm$)	$\langle 2; 3; 9; 5 + (1, 0, 0) \rangle$	$\mathbf{a - b, a + b, c}$	
$C4/mmd$ (127, $P4/mbm$)	$\langle 2; 5; 9; 3 + (1, 0, 0) \rangle$	$\mathbf{a - b, a + b, c}$	1/2, 1/2, 0
$C4/emd$ (125, $P4/nbm$)	$\langle 2; 3; 5; 9 + (1, 0, 0) \rangle$	$\mathbf{a - b, a + b, c}$	1/2, 0, 0
$C4/emd$ (125, $P4/nbm$)	$\langle 2; (3; 5) + (1, 0, 0); 9 + (0, 1, 0) \rangle$	$\mathbf{a - b, a + b, c}$	0, 1/2, 0
$C4/mmm$ (123, $P4/mmm$)	$\langle 2; 3; 5; 9 \rangle$	$\mathbf{a - b, a + b, c}$	
$C4/mmm$ (123, $P4/mmm$)	$\langle (2; 9) + (1, 1, 0); (3; 5) + (1, 0, 0) \rangle$	$\mathbf{a - b, a + b, c}$	1/2, 1/2, 0
[2] $\mathbf{a}' = 2\mathbf{a}, \mathbf{b}' = 2\mathbf{b}, \mathbf{c}' = 2\mathbf{c}$			
$F4/mmc$ (140, $I4/mcm$)	$\langle 2; 3; 9; 5 + (0, 0, 1) \rangle$	$\mathbf{a - b, a + b, 2c}$	
$F4/mmc$ (140, $I4/mcm$)	$\langle 2; 3; 5; 9 + (0, 0, 1) \rangle$	$\mathbf{a - b, a + b, 2c}$	0, 0, 1/2
$F4/mmc$ (140, $I4/mcm$)	$\langle 2; 5; 9; 3 + (0, 0, 1) \rangle$	$\mathbf{a - b, a + b, 2c}$	1/2, 1/2, 0
$F4/mmc$ (140, $I4/mcm$)	$\langle 2; (3; 5; 9) + (0, 0, 1) \rangle$	$\mathbf{a - b, a + b, 2c}$	1/2, 1/2, 1/2
$F4/mmm$ (139, $I4/mmm$)	$\langle 2; 3; 5; 9 \rangle$	$\mathbf{a - b, a + b, 2c}$	
$F4/mmm$ (139, $I4/mmm$)	$\langle 2; 3; (5; 9) + (0, 0, 1) \rangle$	$\mathbf{a - b, a + b, 2c}$	0, 0, 1/2
$F4/mmm$ (139, $I4/mmm$)	$\langle 2; 9; (3; 5) + (0, 0, 1) \rangle$	$\mathbf{a - b, a + b, 2c}$	1/2, 1/2, 0
$F4/mmm$ (139, $I4/mmm$)	$\langle 2; 5; (3; 9) + (0, 0, 1) \rangle$	$\mathbf{a - b, a + b, 2c}$	1/2, 1/2, 1/2
[3] $\mathbf{c}' = 3\mathbf{c}$			
$P4/mmm$ (123)	$\langle 2; 3; 5; 9 \rangle$	$\mathbf{a, b, 3c}$	
$P4/mmm$ (123)	$\langle 2; 3; (5; 9) + (0, 0, 2) \rangle$	$\mathbf{a, b, 3c}$	0, 0, 1
$P4/mmm$ (123)	$\langle 2; 3; (5; 9) + (0, 0, 4) \rangle$	$\mathbf{a, b, 3c}$	0, 0, 2
• Series of maximal isomorphic subgroups			
[p] $\mathbf{c}' = p\mathbf{c}$			
$P4/mmm$ (123)	$\langle 2; 3; (5; 9) + (0, 0, 2u) \rangle$ $p > 2; 0 \leq u < p$ p conjugate subgroups for the prime p	$\mathbf{a, b, pc}$	0, 0, u
[p^2] $\mathbf{a}' = p\mathbf{a}, \mathbf{b}' = p\mathbf{b}$			
$P4/mmm$ (123)	$\langle (2; 9) + (2u, 2v, 0); 3 + (u + v, -u + v, 0); 5 + (2u, 0, 0) \rangle$ $p > 2; 0 \leq u < p; 0 \leq v < p$ p^2 conjugate subgroups for the prime p	$\mathbf{pa, pb, c}$	$u, v, 0$

I Minimal *translationengleiche* supergroups[3] $Pm\bar{3}m$ (221)**II Minimal non-isomorphic *klassengleiche* supergroups**

- **Additional centring translations**

[2] $I4/mmm$ (139)

- **Decreased unit cell**

none