

$Pm\bar{3}m$

No. 221

$P4/m\bar{3}2/m$

$O_h^1$

Generators selected (1);  $t(1,0,0)$ ;  $t(0,1,0)$ ;  $t(0,0,1)$ ; (2); (3); (5); (13); (25)

General position

Multiplicity,  
Wyckoff letter,  
Site symmetry

Coordinates

48	$n$	1	(1) $x, y, z$	(2) $\bar{x}, \bar{y}, z$	(3) $\bar{x}, y, \bar{z}$	(4) $x, \bar{y}, \bar{z}$	(5) $z, x, y$	(6) $z, \bar{x}, \bar{y}$	(7) $\bar{z}, \bar{x}, y$	(8) $\bar{z}, x, \bar{y}$
			(9) $y, z, x$	(10) $\bar{y}, z, \bar{x}$	(11) $y, \bar{z}, \bar{x}$	(12) $\bar{y}, \bar{z}, x$	(13) $y, x, \bar{z}$	(14) $\bar{y}, \bar{x}, \bar{z}$	(15) $y, \bar{x}, z$	(16) $\bar{y}, x, z$
			(17) $x, z, \bar{y}$	(18) $\bar{x}, z, y$	(19) $\bar{x}, \bar{z}, \bar{y}$	(20) $x, \bar{z}, y$	(21) $z, y, \bar{x}$	(22) $z, \bar{y}, x$	(23) $\bar{z}, y, x$	(24) $\bar{z}, \bar{y}, \bar{x}$
			(25) $\bar{x}, \bar{y}, \bar{z}$	(26) $x, y, \bar{z}$	(27) $x, \bar{y}, z$	(28) $\bar{x}, y, z$	(29) $\bar{z}, \bar{x}, \bar{y}$	(30) $\bar{z}, x, y$	(31) $z, x, \bar{y}$	(32) $z, \bar{x}, y$
			(33) $\bar{y}, \bar{z}, \bar{x}$	(34) $y, \bar{z}, x$	(35) $\bar{y}, z, x$	(36) $y, z, \bar{x}$	(37) $\bar{y}, \bar{x}, z$	(38) $y, x, z$	(39) $\bar{y}, x, \bar{z}$	(40) $y, \bar{x}, \bar{z}$
			(41) $\bar{x}, \bar{z}, y$	(42) $x, \bar{z}, \bar{y}$	(43) $x, z, y$	(44) $\bar{x}, z, \bar{y}$	(45) $\bar{z}, \bar{y}, x$	(46) $\bar{z}, y, \bar{x}$	(47) $z, \bar{y}, \bar{x}$	(48) $z, y, x$

I Maximal translationengleiche subgroups

[2] $P\bar{4}3m$ (215)	1; 2; 3; 4; 5; 6; 7; 8; 9; 10; 11; 12; 37; 38; 39; 40; 41; 42; 43; 44; 45; 46; 47; 48	
[2] $P432$ (207)	1; 2; 3; 4; 5; 6; 7; 8; 9; 10; 11; 12; 13; 14; 15; 16; 17; 18; 19; 20; 21; 22; 23; 24	
[2] $Pm\bar{3}1$ (200, $Pm\bar{3}$ )	1; 2; 3; 4; 5; 6; 7; 8; 9; 10; 11; 12; 25; 26; 27; 28; 29; 30; 31; 32; 33; 34; 35; 36	
[3] $P4/m12/m$ (123, $P4/mmm$ )	1; 2; 3; 4; 13; 14; 15; 16; 25; 26; 27; 28; 37; 38; 39; 40	<b>b, c, a</b> <b>c, a, b</b> <b>a - b, b - c, a + b + c</b> <b>-a - b, b + c, -a + b - c</b> <b>a + b, -b + c, a - b - c</b> <b>-a + b, -b - c, -a - b + c</b>
[3] $P4/m12/m$ (123, $P4/mmm$ )	1; 4; 2; 3; 18; 19; 17; 20; 25; 28; 26; 27; 42; 43; 41; 44	
[3] $P4/m12/m$ (123, $P4/mmm$ )	1; 3; 4; 2; 22; 24; 23; 21; 25; 27; 28; 26; 46; 48; 47; 45	
[4] $P1\bar{3}2/m$ (166, $R\bar{3}m$ )	1; 5; 9; 14; 19; 24; 25; 29; 33; 38; 43; 48	
[4] $P1\bar{3}2/m$ (166, $R\bar{3}m$ )	1; 6; 12; 13; 18; 24; 25; 30; 36; 37; 42; 48	
[4] $P1\bar{3}2/m$ (166, $R\bar{3}m$ )	1; 7; 10; 13; 19; 22; 25; 31; 34; 37; 43; 46	
[4] $P1\bar{3}2/m$ (166, $R\bar{3}m$ )	1; 8; 11; 14; 18; 22; 25; 32; 35; 38; 42; 46	

II Maximal klassengleiche subgroups

• Enlarged unit cell

[2] $\mathbf{a}' = 2\mathbf{a}, \mathbf{b}' = 2\mathbf{b}, \mathbf{c}' = 2\mathbf{c}$		
$Fm\bar{3}m$ (225)	$\langle 2; 3; 5; 13; 25 \rangle$	$2\mathbf{a}, 2\mathbf{b}, 2\mathbf{c}$
$Fm\bar{3}c$ (226)	$\langle 2; 3; 5; 25; 13 + (1, 1, 1) \rangle$	$2\mathbf{a}, 2\mathbf{b}, 2\mathbf{c}$
$Fm\bar{3}c$ (226)	$\langle 2; 3; 5; 13; 25 + (1, 1, 1) \rangle$	$2\mathbf{a}, 2\mathbf{b}, 2\mathbf{c}$ $1/2, 1/2, 1/2$
$Fm\bar{3}m$ (225)	$\langle 2; 3; 5; 13 + (0, 0, 1); 25 + (1, 1, 1) \rangle$	$2\mathbf{a}, 2\mathbf{b}, 2\mathbf{c}$ $1/2, 1/2, 1/2$
[4] $\mathbf{a}' = 2\mathbf{a}, \mathbf{b}' = 2\mathbf{b}, \mathbf{c}' = 2\mathbf{c}$		
$Im\bar{3}m$ (229)	$\langle 2; 3; 5; 13; 25 \rangle$	$2\mathbf{a}, 2\mathbf{b}, 2\mathbf{c}$
$Im\bar{3}m$ (229)	$\langle 13; (2; 25) + (2, 2, 0); 3 + (2, 0, 0); 5 + (1, 0, -1) \rangle$	$2\mathbf{a}, 2\mathbf{b}, 2\mathbf{c}$ $1, 1, 0$
$Im\bar{3}m$ (229)	$\langle (2; 3; 25) + (2, 0, 0); (5; 13) + (1, -1, 0) \rangle$	$2\mathbf{a}, 2\mathbf{b}, 2\mathbf{c}$ $1, 0, 0$
$Im\bar{3}m$ (229)	$\langle 3; (2; 25) + (0, 2, 0); 5 + (0, 1, -1); 13 + (-1, 1, 0) \rangle$	$2\mathbf{a}, 2\mathbf{b}, 2\mathbf{c}$ $0, 1, 0$
$Im\bar{3}m$ (229)	$\langle 5; 25; (2; 13) + (0, 0, 1); 3 + (0, 1, 0) \rangle$	$2\mathbf{a}, 2\mathbf{b}, 2\mathbf{c}$ $1/2, 1/2, 1/2$
$Im\bar{3}m$ (229)	$\langle 2 + (2, 2, 1); 3 + (2, 1, 0); 5 + (1, 0, -1); 13 + (0, 0, 1); 25 + (2, 2, 0) \rangle$	$2\mathbf{a}, 2\mathbf{b}, 2\mathbf{c}$ $3/2, 3/2, 1/2$
$Im\bar{3}m$ (229)	$\langle 2 + (2, 0, 1); 3 + (2, 1, 0); 5 + (1, -1, 0); 13 + (1, -1, 1); 25 + (2, 0, 0) \rangle$	$2\mathbf{a}, 2\mathbf{b}, 2\mathbf{c}$ $3/2, 1/2, 1/2$
$Im\bar{3}m$ (229)	$\langle 2 + (0, 2, 1); 3 + (0, 1, 0); 5 + (0, 1, -1); 13 + (-1, 1, 1); 25 + (0, 2, 0) \rangle$	$2\mathbf{a}, 2\mathbf{b}, 2\mathbf{c}$ $1/2, 3/2, 1/2$

• Series of maximal isomorphic subgroups

[ $p^3$ ] $\mathbf{a}' = p\mathbf{a}, \mathbf{b}' = p\mathbf{b}, \mathbf{c}' = p\mathbf{c}$		
$Pm\bar{3}m$ (221)	$\langle 2 + (2u, 2v, 0); 3 + (2u, 0, 2w); 5 + (u - w, -u + v, -v + w); 13 + (u - v, -u + v, 2w); 25 + (2u, 2v, 2w) \rangle$ $p > 2; 0 \leq u < p; 0 \leq v < p; 0 \leq w < p$ $p^3$ conjugate subgroups for the prime $p$	$p\mathbf{a}, p\mathbf{b}, p\mathbf{c}$ $u, v, w$

I Minimal translationengleiche supergroups

none

II Minimal non-isomorphic klassengleiche supergroups

• Additional centring translations

[2]  $Im\bar{3}m$  (229); [4]  $Fm\bar{3}m$  (225)

• Decreased unit cell

none