

$P4/mnc$

D_{4h}^6

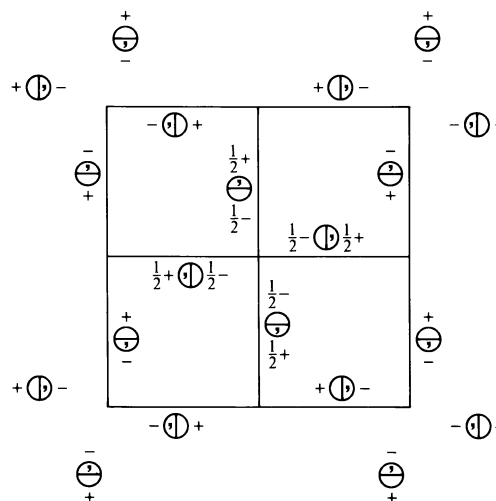
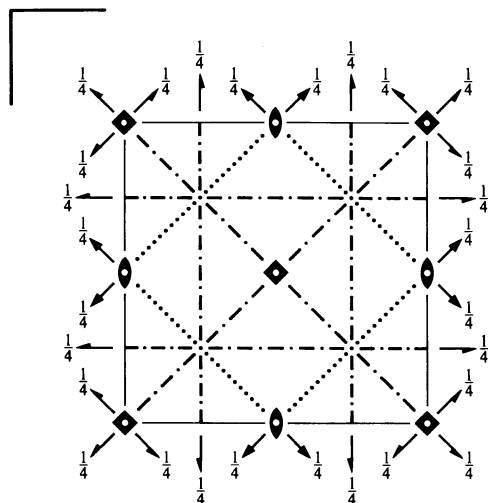
$4/mmm$

Tetragonal

No. 128

$P 4/m 2_1/n 2/c$

Patterson symmetry $P4/mmm$



Origin at centre ($4/m$) at $4/m1n$

Asymmetric unit $0 \leq x \leq \frac{1}{2}; 0 \leq y \leq \frac{1}{2}; 0 \leq z \leq \frac{1}{4}$

Symmetry operations

- | | | | |
|---|---|--|---|
| (1) 1 | (2) $2 \ 0,0,z$ | (3) $4^+ \ 0,0,z$ | (4) $4^- \ 0,0,z$ |
| (5) $2(0, \frac{1}{2}, 0) \ \frac{1}{4}, y, \frac{1}{4}$ | (6) $2(\frac{1}{2}, 0, 0) \ x, \frac{1}{4}, \frac{1}{4}$ | (7) $2(\frac{1}{2}, \frac{1}{2}, 0) \ x, x, \frac{1}{4}$ | (8) $2 \ x, \bar{x} + \frac{1}{2}, \frac{1}{4}$ |
| (9) $\bar{1} \ 0,0,0$ | (10) $m \ x,y,0$ | (11) $4^+ \ 0,0,z; \ 0,0,0$ | (12) $4^- \ 0,0,z; \ 0,0,0$ |
| (13) $n(\frac{1}{2}, 0, \frac{1}{2}) \ x, \frac{1}{4}, z$ | (14) $n(0, \frac{1}{2}, \frac{1}{2}) \ \frac{1}{4}, y, z$ | (15) $c \ x + \frac{1}{2}, \bar{x}, z$ | (16) $n(\frac{1}{2}, \frac{1}{2}, \frac{1}{2}) \ x, x, z$ |

Generators selected (1); $t(1,0,0)$; $t(0,1,0)$; $t(0,0,1)$; (2); (3); (5); (9)

Positions

Multiplicity, Wyckoff letter, Site symmetry	Coordinates	Reflection conditions
		General:
16 <i>i</i> 1	(1) x, y, z (5) $\bar{x} + \frac{1}{2}, y + \frac{1}{2}, \bar{z} + \frac{1}{2}$ (9) $\bar{x}, \bar{y}, \bar{z}$ (13) $x + \frac{1}{2}, \bar{y} + \frac{1}{2}, z + \frac{1}{2}$	$0kl : k + l = 2n$ $hhl : l = 2n$ $00l : l = 2n$ $h00 : h = 2n$
	(2) \bar{x}, \bar{y}, z (6) $x + \frac{1}{2}, \bar{y} + \frac{1}{2}, \bar{z} + \frac{1}{2}$ (10) x, y, \bar{z} (14) $\bar{x} + \frac{1}{2}, y + \frac{1}{2}, z + \frac{1}{2}$	
	(3) \bar{y}, x, z (7) $y + \frac{1}{2}, x + \frac{1}{2}, \bar{z} + \frac{1}{2}$ (11) y, \bar{x}, \bar{z} (15) $\bar{y} + \frac{1}{2}, \bar{x} + \frac{1}{2}, z + \frac{1}{2}$	
	(4) y, \bar{x}, z (8) $\bar{y} + \frac{1}{2}, \bar{x} + \frac{1}{2}, \bar{z} + \frac{1}{2}$ (12) \bar{y}, x, \bar{z} (16) $y + \frac{1}{2}, x + \frac{1}{2}, z + \frac{1}{2}$	
		Special: as above, plus
8 <i>h</i> $m..$	$x, y, 0$ $\bar{x} + \frac{1}{2}, y + \frac{1}{2}, \frac{1}{2}$	$\bar{x}, \bar{y}, 0$ $x + \frac{1}{2}, \bar{y} + \frac{1}{2}, \frac{1}{2}$
	$\bar{y}, x, 0$ $y + \frac{1}{2}, x + \frac{1}{2}, \frac{1}{2}$	$y, \bar{x}, 0$ $\bar{y} + \frac{1}{2}, \bar{x} + \frac{1}{2}, \frac{1}{2}$
		no extra conditions
8 <i>g</i> $..2$	$x, x + \frac{1}{2}, \frac{1}{4}$ $\bar{x}, \bar{x} + \frac{1}{2}, \frac{3}{4}$	$\bar{x}, \bar{x} + \frac{1}{2}, \frac{1}{4}$ $x, x + \frac{1}{2}, \frac{3}{4}$
	$\bar{x} + \frac{1}{2}, x, \frac{1}{4}$ $x + \frac{1}{2}, \bar{x}, \frac{3}{4}$	$x + \frac{1}{2}, \bar{x}, \frac{1}{4}$ $\bar{x} + \frac{1}{2}, x, \frac{3}{4}$
		$hkl : l = 2n$
8 <i>f</i> $2..$	$0, \frac{1}{2}, z$ $0, \frac{1}{2}, \bar{z}$	$\frac{1}{2}, 0, z$ $\frac{1}{2}, 0, \bar{z}$
	$\frac{1}{2}, 0, \bar{z} + \frac{1}{2}$ $\frac{1}{2}, 0, z + \frac{1}{2}$	$0, \frac{1}{2}, \bar{z} + \frac{1}{2}$ $0, \frac{1}{2}, z + \frac{1}{2}$
		$hkl : h + k, l = 2n$
4 <i>e</i> $4..$	$0, 0, z$	$\frac{1}{2}, \frac{1}{2}, \bar{z} + \frac{1}{2}$ $0, 0, \bar{z}$ $\frac{1}{2}, \frac{1}{2}, z + \frac{1}{2}$
		$hkl : h + k + l = 2n$
4 <i>d</i> 2.22	$0, \frac{1}{2}, \frac{1}{4}$	$\frac{1}{2}, 0, \frac{1}{4}$ $0, \frac{1}{2}, \frac{3}{4}$ $\frac{1}{2}, 0, \frac{3}{4}$
		$hkl : h + k, l = 2n$
4 <i>c</i> $2/m..$	$0, \frac{1}{2}, 0$	$\frac{1}{2}, 0, 0$ $\frac{1}{2}, 0, \frac{1}{2}$ $0, \frac{1}{2}, \frac{1}{2}$
		$hkl : h + k, l = 2n$
2 <i>b</i> $4/m..$	$0, 0, \frac{1}{2}$	$\frac{1}{2}, \frac{1}{2}, 0$
		$hkl : h + k + l = 2n$
2 <i>a</i> $4/m..$	$0, 0, 0$	$\frac{1}{2}, \frac{1}{2}, \frac{1}{2}$
		$hkl : h + k + l = 2n$

Symmetry of special projections

Along [001] $p4gm$
 $\mathbf{a}' = \mathbf{a}$ $\mathbf{b}' = \mathbf{b}$
Origin at $0, 0, z$

Along [100] $c2mm$
 $\mathbf{a}' = \mathbf{b}$ $\mathbf{b}' = \mathbf{c}$
Origin at $x, 0, 0$

Along [110] $p2mm$
 $\mathbf{a}' = \frac{1}{2}(-\mathbf{a} + \mathbf{b})$ $\mathbf{b}' = \frac{1}{2}\mathbf{c}$
Origin at $x, x, 0$

Maximal non-isomorphic subgroups

I	[2] $P\bar{4}n2$ (118)	1; 2; 7; 8; 11; 12; 13; 14
	[2] $P\bar{4}2_1c$ (114)	1; 2; 5; 6; 11; 12; 15; 16
	[2] $P4nc$ (104)	1; 2; 3; 4; 13; 14; 15; 16
	[2] $P4_22$ (90)	1; 2; 3; 4; 5; 6; 7; 8
	[2] $P4/m11$ ($P4/m$, 83)	1; 2; 3; 4; 9; 10; 11; 12
	[2] $P2/m12/c$ ($Cccm$, 66)	1; 2; 7; 8; 9; 10; 15; 16
	[2] $P2/m2_1/n1$ ($Pnnm$, 58)	1; 2; 5; 6; 9; 10; 13; 14

IIa none

IIb none

Maximal isomorphic subgroups of lowest index

IIc [3] $P4/mnc$ ($\mathbf{c}' = 3\mathbf{c}$) (128); [9] $P4/mnc$ ($\mathbf{a}' = 3\mathbf{a}, \mathbf{b}' = 3\mathbf{b}$) (128)

Minimal non-isomorphic supergroups

I none

II [2] $C4/mcc$ ($P4/mcc$, 124); [2] $I4/mmm$ (139); [2] $P4/mbm$ ($\mathbf{c}' = \frac{1}{2}\mathbf{c}$) (127)