

$P4/mcc$

D_{4h}^2

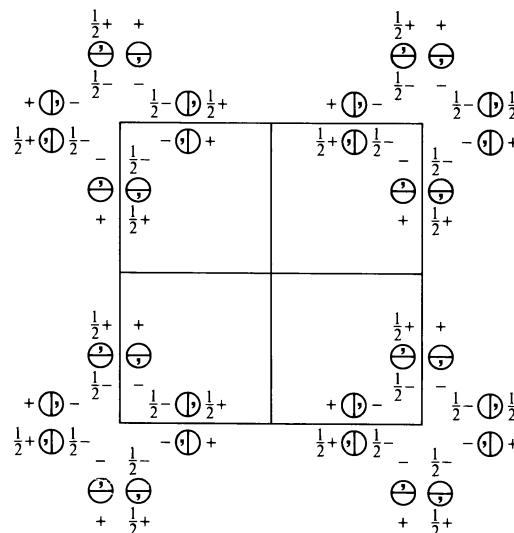
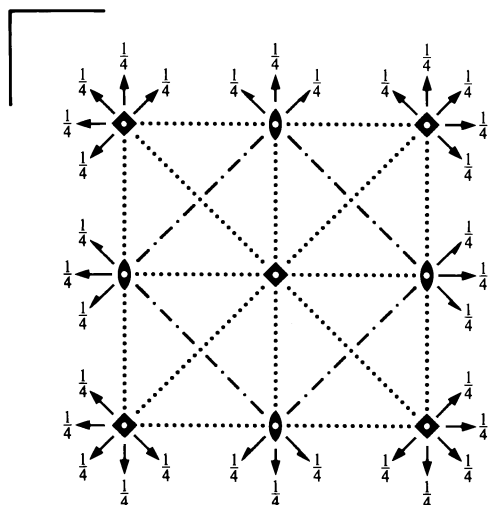
$4/mmm$

Tetragonal

No. 124

$P 4/m 2/c 2/c$

Patterson symmetry $P4/mmm$



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

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

Maximal isomorphic subgroups of lowest index

IIc [2] $C4/mcc$ ($a' = 2a, b' = 2b$) ($P4/mcc$, 124); [3] $P4/mcc$ ($c' = 3c$) (124)

Minimal non-isomorphic supergroups

I none

II [2] $I4/mcm$ (140); [2] $P4/mmm$ ($c' = \frac{1}{2}c$) (123)

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
16 <i>n</i> 1	(1) x, y, z (5) $\bar{x}, y, \bar{z} + \frac{1}{2}$ (9) $\bar{x}, \bar{y}, \bar{z}$ (13) $x, \bar{y}, z + \frac{1}{2}$	(2) \bar{x}, \bar{y}, z (6) $x, \bar{y}, \bar{z} + \frac{1}{2}$ (10) x, y, \bar{z} (14) $\bar{x}, y, z + \frac{1}{2}$	(3) \bar{y}, x, z (7) $y, x, \bar{z} + \frac{1}{2}$ (11) y, \bar{x}, \bar{z} (15) $\bar{y}, \bar{x}, z + \frac{1}{2}$	(4) y, \bar{x}, z (8) $\bar{y}, \bar{x}, \bar{z} + \frac{1}{2}$ (12) \bar{y}, x, \bar{z} (16) $y, x, z + \frac{1}{2}$	General: $0kl : l = 2n$ $hhl : l = 2n$ $00l : l = 2n$ Special: as above, plus no extra conditions
8 <i>m</i> <i>m</i> ..	$x, y, 0$ $\bar{x}, y, \frac{1}{2}$	$\bar{x}, \bar{y}, 0$ $x, \bar{y}, \frac{1}{2}$	$\bar{y}, x, 0$ $y, x, \frac{1}{2}$	$y, \bar{x}, 0$ $\bar{y}, \bar{x}, \frac{1}{2}$	
8 <i>l</i> .2.	$x, \frac{1}{2}, \frac{1}{4}$ $\bar{x}, \frac{1}{2}, \frac{3}{4}$	$\bar{x}, \frac{1}{2}, \frac{1}{4}$ $x, \frac{1}{2}, \frac{3}{4}$	$\frac{1}{2}, x, \frac{1}{4}$ $\frac{1}{2}, \bar{x}, \frac{3}{4}$	$\frac{1}{2}, \bar{x}, \frac{1}{4}$ $\frac{1}{2}, x, \frac{3}{4}$	$hkl : l = 2n$
8 <i>k</i> .2.	$x, 0, \frac{1}{4}$ $\bar{x}, 0, \frac{3}{4}$	$\bar{x}, 0, \frac{1}{4}$ $x, 0, \frac{3}{4}$	$0, x, \frac{1}{4}$ $0, \bar{x}, \frac{3}{4}$	$0, \bar{x}, \frac{1}{4}$ $0, x, \frac{3}{4}$	$hkl : l = 2n$
8 <i>j</i> ..2	$x, x, \frac{1}{4}$ $\bar{x}, \bar{x}, \frac{3}{4}$	$\bar{x}, \bar{x}, \frac{1}{4}$ $x, x, \frac{3}{4}$	$\bar{x}, x, \frac{1}{4}$ $x, \bar{x}, \frac{3}{4}$	$x, \bar{x}, \frac{1}{4}$ $\bar{x}, x, \frac{3}{4}$	$hkl : l = 2n$
8 <i>i</i> 2..	$0, \frac{1}{2}, z$ $0, \frac{1}{2}, \bar{z}$	$\frac{1}{2}, 0, z$ $\frac{1}{2}, 0, \bar{z}$	$0, \frac{1}{2}, \bar{z} + \frac{1}{2}$ $0, \frac{1}{2}, z + \frac{1}{2}$	$\frac{1}{2}, 0, \bar{z} + \frac{1}{2}$ $\frac{1}{2}, 0, z + \frac{1}{2}$	$hkl : h + k, l = 2n$
4 <i>h</i> 4..	$\frac{1}{2}, \frac{1}{2}, z$	$\frac{1}{2}, \frac{1}{2}, \bar{z} + \frac{1}{2}$	$\frac{1}{2}, \frac{1}{2}, \bar{z}$	$\frac{1}{2}, \frac{1}{2}, z + \frac{1}{2}$	$hkl : l = 2n$
4 <i>g</i> 4..	$0, 0, z$	$0, 0, \bar{z} + \frac{1}{2}$	$0, 0, \bar{z}$	$0, 0, z + \frac{1}{2}$	$hkl : l = 2n$
4 <i>f</i> 222.	$0, \frac{1}{2}, \frac{1}{4}$	$\frac{1}{2}, 0, \frac{1}{4}$	$0, \frac{1}{2}, \frac{3}{4}$	$\frac{1}{2}, 0, \frac{3}{4}$	$hkl : h + k, l = 2n$
4 <i>e</i> 2/m..	$0, \frac{1}{2}, 0$	$\frac{1}{2}, 0, 0$	$0, \frac{1}{2}, \frac{1}{2}$	$\frac{1}{2}, 0, \frac{1}{2}$	$hkl : h + k, l = 2n$
2 <i>d</i> 4/m..	$\frac{1}{2}, \frac{1}{2}, 0$	$\frac{1}{2}, \frac{1}{2}, \frac{1}{2}$			$hkl : l = 2n$
2 <i>c</i> 422	$\frac{1}{2}, \frac{1}{2}, \frac{1}{4}$	$\frac{1}{2}, \frac{1}{2}, \frac{3}{4}$			$hkl : l = 2n$
2 <i>b</i> 4/m..	$0, 0, 0$	$0, 0, \frac{1}{2}$			$hkl : l = 2n$
2 <i>a</i> 422	$0, 0, \frac{1}{4}$	$0, 0, \frac{3}{4}$			$hkl : l = 2n$

Symmetry of special projections

Along [001] $p4mm$
 $\mathbf{a}' = \mathbf{a}$ $\mathbf{b}' = \mathbf{b}$
Origin at $0, 0, z$

Along [100] $p2mm$
 $\mathbf{a}' = \mathbf{b}$ $\mathbf{b}' = \frac{1}{2}\mathbf{c}$
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] $P\bar{4}c2$ (116)	1; 2; 7; 8; 11; 12; 13; 14
	[2] $P\bar{4}2c$ (112)	1; 2; 5; 6; 11; 12; 15; 16
	[2] $P4cc$ (103)	1; 2; 3; 4; 13; 14; 15; 16
	[2] $P422$ (89)	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] $P2/m2/c1$ ($Pccm$, 49)	1; 2; 5; 6; 9; 10; 13; 14

IIa none

IIb [2] $C4/ecc$ ($\mathbf{a}' = 2\mathbf{a}, \mathbf{b}' = 2\mathbf{b}$) ($P4/ncc$, 130); [2] $C4/mcd$ ($\mathbf{a}' = 2\mathbf{a}, \mathbf{b}' = 2\mathbf{b}$) ($P4/mnc$, 128);
[2] $C4/ecd$ ($\mathbf{a}' = 2\mathbf{a}, \mathbf{b}' = 2\mathbf{b}$) ($P4/nnc$, 126)

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