

$P4/mmm$

D_{4h}^1

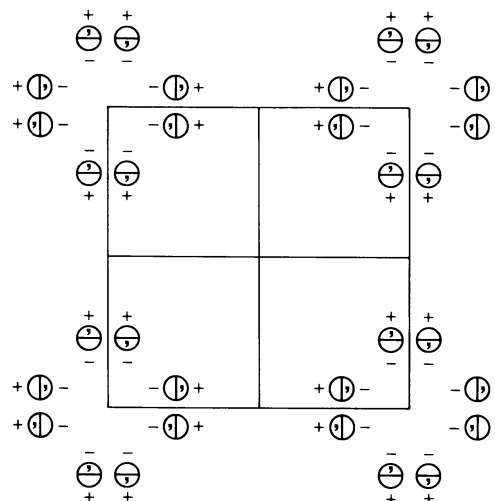
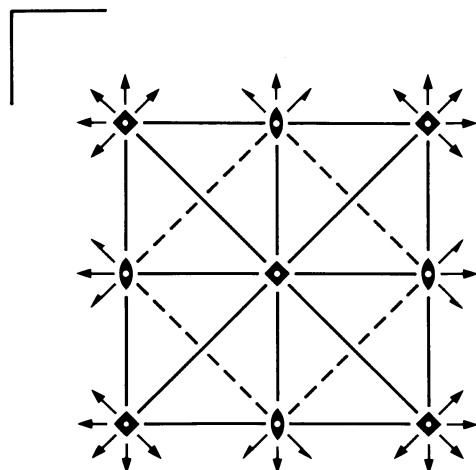
$4/mmm$

Tetragonal

No. 123

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

Patterson symmetry $P4/mmm$



Origin at centre ($4/mmm$)

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

Symmetry operations

- | | | | |
|---------------------|--------------|-------------------------------|-------------------------------|
| (1) 1 | (2) 2 0,0,z | (3) 4 ⁺ 0,0,z | (4) 4 ⁻ 0,0,z |
| (5) 2 0,y,0 | (6) 2 x,0,0 | (7) 2 x,x,0 | (8) 2 x,x̄,0 |
| (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) m x,0,z | (14) m 0,y,z | (15) m x,x̄,z | (16) m x,x,z |

Maximal non-isomorphic subgroups

- I** [2] $P\bar{4}m2$ (115) 1; 2; 7; 8; 11; 12; 13; 14
 [2] $P\bar{4}2m$ (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] $P4/m11$ ($P4/m$, 83) 1; 2; 3; 4; 9; 10; 11; 12
 [2] $P2/m12/m$ ($Cmmm$, 65) 1; 2; 7; 8; 9; 10; 15; 16
 [2] $P2/m2/m1$ ($Pmmm$, 47) 1; 2; 5; 6; 9; 10; 13; 14

IIa none

- IIb** [2] $P4_2/mcm$ ($c' = 2c$) (132); [2] $P4_2/mmc$ ($c' = 2c$) (131); [2] $P4/mcc$ ($c' = 2c$) (124);
 [2] $C4/emm$ ($a' = 2a, b' = 2b$) ($P4/nmm$, 129); [2] $C4/mmd$ ($a' = 2a, b' = 2b$) ($P4/mbm$, 127);
 [2] $C4/emd$ ($a' = 2a, b' = 2b$) ($P4/nbm$, 125); [2] $F4/mmc$ ($a' = 2a, b' = 2b, c' = 2c$) ($I4/mcm$, 140);
 [2] $F4/mmm$ ($a' = 2a, b' = 2b, c' = 2c$) ($I4/mmm$, 139)

Maximal isomorphic subgroups of lowest index

- IIc** [2] $P4/mmm$ ($c' = 2c$) (123); [2] $C4/mmm$ ($a' = 2a, b' = 2b$) ($P4/mmm$, 123)

Minimal non-isomorphic supergroups

- I** [3] $Pm\bar{3}m$ (221)
II [2] $I4/mmm$ (139)

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>u</i> 1	(1) x, y, z (5) \bar{x}, y, \bar{z} (9) $\bar{x}, \bar{y}, \bar{z}$ (13) x, \bar{y}, z	(2) \bar{x}, \bar{y}, z (6) x, \bar{y}, \bar{z} (10) x, y, \bar{z} (14) \bar{x}, y, z	(3) \bar{y}, x, z (7) y, x, \bar{z} (11) y, \bar{x}, \bar{z} (15) \bar{y}, \bar{x}, z	(4) y, \bar{x}, z (8) $\bar{y}, \bar{x}, \bar{z}$ (12) \bar{y}, x, \bar{z} (16) y, x, z	General: no conditions
8	<i>t</i> . <i>m</i> .	$x, \frac{1}{2}, z$ $\bar{x}, \frac{1}{2}, \bar{z}$	$\bar{x}, \frac{1}{2}, z$ $x, \frac{1}{2}, \bar{z}$	$\frac{1}{2}, x, z$ $\frac{1}{2}, x, \bar{z}$	$\frac{1}{2}, \bar{x}, z$ $\frac{1}{2}, \bar{x}, \bar{z}$	Special: no extra conditions
8	<i>s</i> . <i>m</i> .	$x, 0, z$ $\bar{x}, 0, \bar{z}$	$\bar{x}, 0, z$ $x, 0, \bar{z}$	$0, x, z$ $0, x, \bar{z}$	$0, \bar{x}, z$ $0, \bar{x}, \bar{z}$	no extra conditions
8	<i>r</i> . . <i>m</i>	x, x, z \bar{x}, x, \bar{z}	\bar{x}, \bar{x}, z x, \bar{x}, \bar{z}	\bar{x}, x, z x, x, \bar{z}	x, \bar{x}, z $\bar{x}, \bar{x}, \bar{z}$	no extra conditions
8	<i>q</i> <i>m</i> . .	$x, y, \frac{1}{2}$ $\bar{x}, y, \frac{1}{2}$	$\bar{x}, \bar{y}, \frac{1}{2}$ $x, \bar{y}, \frac{1}{2}$	$\bar{y}, x, \frac{1}{2}$ $y, x, \frac{1}{2}$	$y, \bar{x}, \frac{1}{2}$ $\bar{y}, \bar{x}, \frac{1}{2}$	no extra conditions
8	<i>p</i> <i>m</i> . .	$x, y, 0$ $\bar{x}, y, 0$	$\bar{x}, \bar{y}, 0$ $x, \bar{y}, 0$	$\bar{y}, x, 0$ $y, x, 0$	$y, \bar{x}, 0$ $\bar{y}, \bar{x}, 0$	no extra conditions
4	<i>o</i> <i>m</i> 2 <i>m</i> .	$x, \frac{1}{2}, \frac{1}{2}$	$\bar{x}, \frac{1}{2}, \frac{1}{2}$	$\frac{1}{2}, x, \frac{1}{2}$	$\frac{1}{2}, \bar{x}, \frac{1}{2}$	no extra conditions
4	<i>n</i> <i>m</i> 2 <i>m</i> .	$x, \frac{1}{2}, 0$	$\bar{x}, \frac{1}{2}, 0$	$\frac{1}{2}, x, 0$	$\frac{1}{2}, \bar{x}, 0$	no extra conditions
4	<i>m</i> <i>m</i> 2 <i>m</i> .	$x, 0, \frac{1}{2}$	$\bar{x}, 0, \frac{1}{2}$	$0, x, \frac{1}{2}$	$0, \bar{x}, \frac{1}{2}$	no extra conditions
4	<i>l</i> <i>m</i> 2 <i>m</i> .	$x, 0, 0$	$\bar{x}, 0, 0$	$0, x, 0$	$0, \bar{x}, 0$	no extra conditions
4	<i>k</i> <i>m</i> . 2 <i>m</i>	$x, x, \frac{1}{2}$	$\bar{x}, \bar{x}, \frac{1}{2}$	$\bar{x}, x, \frac{1}{2}$	$x, \bar{x}, \frac{1}{2}$	no extra conditions
4	<i>j</i> <i>m</i> . 2 <i>m</i>	$x, x, 0$	$\bar{x}, \bar{x}, 0$	$\bar{x}, x, 0$	$x, \bar{x}, 0$	no extra conditions
4	<i>i</i> 2 <i>m m</i> .	$0, \frac{1}{2}, z$	$\frac{1}{2}, 0, z$	$0, \frac{1}{2}, \bar{z}$	$\frac{1}{2}, 0, \bar{z}$	$hkl : h + k = 2n$
2	<i>h</i> 4 <i>m m</i>	$\frac{1}{2}, \frac{1}{2}, z$	$\frac{1}{2}, \frac{1}{2}, \bar{z}$			no extra conditions
2	<i>g</i> 4 <i>m m</i>	$0, 0, z$	$0, 0, \bar{z}$			no extra conditions
2	<i>f</i> <i>m m m</i> .	$0, \frac{1}{2}, 0$	$\frac{1}{2}, 0, 0$			$hkl : h + k = 2n$
2	<i>e</i> <i>m m m</i> .	$0, \frac{1}{2}, \frac{1}{2}$	$\frac{1}{2}, 0, \frac{1}{2}$			$hkl : h + k = 2n$
1	<i>d</i> 4/ <i>m m m</i>	$\frac{1}{2}, \frac{1}{2}, \frac{1}{2}$				no extra conditions
1	<i>c</i> 4/ <i>m m m</i>	$\frac{1}{2}, \frac{1}{2}, 0$				no extra conditions
1	<i>b</i> 4/ <i>m m m</i>	$0, 0, \frac{1}{2}$				no extra conditions
1	<i>a</i> 4/ <i>m m m</i>	$0, 0, 0$				no extra conditions

Symmetry of special projectionsAlong [001] $p4mm$ $\mathbf{a}' = \mathbf{a}$ $\mathbf{b}' = \mathbf{b}$

Origin at 0, 0, z

Along [100] $p2mm$ $\mathbf{a}' = \mathbf{b}$ $\mathbf{b}' = \mathbf{c}$ Origin at $x, 0, 0$ Along [110] $p2mm$ $\mathbf{a}' = \frac{1}{2}(-\mathbf{a} + \mathbf{b})$ $\mathbf{b}' = \mathbf{c}$ Origin at $x, x, 0$

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