

$P4/nbm$

D_{4h}^3

$4/mmm$

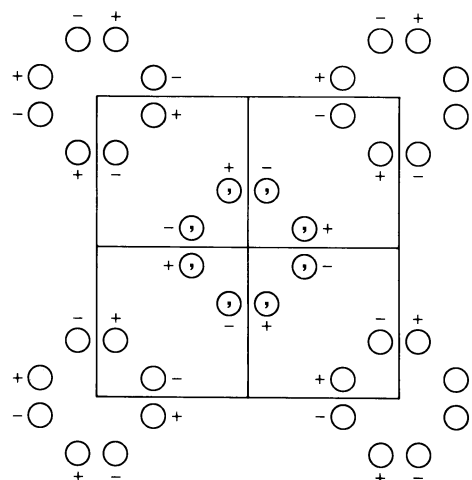
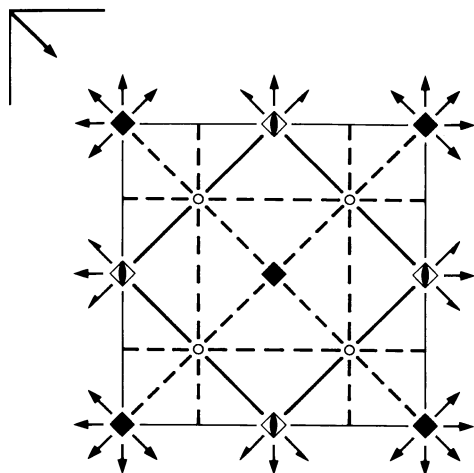
Tetragonal

No. 125

$P 4/n 2/b 2/m$

Patterson symmetry $P4/mmm$

ORIGIN CHOICE 1



Origin at 422 at $4/n22/g$, at $-\frac{1}{4}, -\frac{1}{4}, 0$ from centre ($2/m$)

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

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 $x, \bar{x}, 0$ |
| (9) $\bar{1}$ $\frac{1}{4}, \frac{1}{4}, 0$ | (10) $n(\frac{1}{2}, \frac{1}{2}, 0)$ $x, y, 0$ | (11) $\bar{4}^+$ $\frac{1}{2}, 0, z; \frac{1}{2}, 0, 0$ | (12) $\bar{4}^-$ $0, \frac{1}{2}, z; 0, \frac{1}{2}, 0$ |
| (13) a $x, \frac{1}{4}, z$ | (14) b $\frac{1}{4}, y, z$ | (15) m $x + \frac{1}{2}, \bar{x}, z$ | (16) $g(\frac{1}{2}, \frac{1}{2}, 0)$ x, x, z |

Maximal isomorphic subgroups of lowest index

IIc [2] $P4/nbm$ ($c' = 2c$) (125); [9] $P4/nbm$ ($a' = 3a, b' = 3b$) (125)

Minimal non-isomorphic supergroups

I none

II [2] $C4/mmm$ ($P4/mmm$, 123); [2] $I4/mcm$ (140)

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 n 1	(1) x, y, z (5) \bar{x}, y, \bar{z} (9) $\bar{x} + \frac{1}{2}, \bar{y} + \frac{1}{2}, \bar{z}$ (13) $x + \frac{1}{2}, \bar{y} + \frac{1}{2}, z$	(2) \bar{x}, \bar{y}, z (6) x, \bar{y}, \bar{z} (10) $x + \frac{1}{2}, y + \frac{1}{2}, \bar{z}$ (14) $\bar{x} + \frac{1}{2}, y + \frac{1}{2}, z$	(3) \bar{y}, x, z (7) y, x, \bar{z} (11) $y + \frac{1}{2}, \bar{x} + \frac{1}{2}, \bar{z}$ (15) $\bar{y} + \frac{1}{2}, \bar{x} + \frac{1}{2}, z$	(4) y, \bar{x}, z (8) $\bar{y}, \bar{x}, \bar{z}$ (12) $\bar{y} + \frac{1}{2}, x + \frac{1}{2}, \bar{z}$ (16) $y + \frac{1}{2}, x + \frac{1}{2}, z$	$hk0 : h + k = 2n$ $0kl : k = 2n$ $h00 : h = 2n$
					Special: as above, plus
8 m . . m	$x, x + \frac{1}{2}, z$ $\bar{x}, x + \frac{1}{2}, \bar{z}$	$\bar{x}, \bar{x} + \frac{1}{2}, z$ $x, \bar{x} + \frac{1}{2}, \bar{z}$	$\bar{x} + \frac{1}{2}, x, z$ $x + \frac{1}{2}, x, \bar{z}$	$x + \frac{1}{2}, \bar{x}, z$ $\bar{x} + \frac{1}{2}, \bar{x}, \bar{z}$	no extra conditions
8 l . 2 .	$x, 0, \frac{1}{2}$ $\bar{x} + \frac{1}{2}, \frac{1}{2}, \frac{1}{2}$	$\bar{x}, 0, \frac{1}{2}$ $x + \frac{1}{2}, \frac{1}{2}, \frac{1}{2}$	$0, x, \frac{1}{2}$ $\frac{1}{2}, \bar{x} + \frac{1}{2}, \frac{1}{2}$	$0, \bar{x}, \frac{1}{2}$ $\frac{1}{2}, x + \frac{1}{2}, \frac{1}{2}$	$hkl : h + k = 2n$
8 k . 2 .	$x, 0, 0$ $\bar{x} + \frac{1}{2}, \frac{1}{2}, 0$	$\bar{x}, 0, 0$ $x + \frac{1}{2}, \frac{1}{2}, 0$	$0, x, 0$ $\frac{1}{2}, \bar{x} + \frac{1}{2}, 0$	$0, \bar{x}, 0$ $\frac{1}{2}, x + \frac{1}{2}, 0$	$hkl : h + k = 2n$
8 j . . 2	$x, x, \frac{1}{2}$ $\bar{x} + \frac{1}{2}, \bar{x} + \frac{1}{2}, \frac{1}{2}$	$\bar{x}, \bar{x}, \frac{1}{2}$ $x + \frac{1}{2}, x + \frac{1}{2}, \frac{1}{2}$	$\bar{x}, x, \frac{1}{2}$ $x + \frac{1}{2}, \bar{x} + \frac{1}{2}, \frac{1}{2}$	$x, \bar{x}, \frac{1}{2}$ $\bar{x} + \frac{1}{2}, x + \frac{1}{2}, \frac{1}{2}$	$hkl : h + k = 2n$
8 i . . 2	$x, x, 0$ $\bar{x} + \frac{1}{2}, \bar{x} + \frac{1}{2}, 0$	$\bar{x}, \bar{x}, 0$ $x + \frac{1}{2}, x + \frac{1}{2}, 0$	$\bar{x}, x, 0$ $x + \frac{1}{2}, \bar{x} + \frac{1}{2}, 0$	$x, \bar{x}, 0$ $\bar{x} + \frac{1}{2}, x + \frac{1}{2}, 0$	$hkl : h + k = 2n$
4 h 2 . mm	$0, \frac{1}{2}, z$	$\frac{1}{2}, 0, z$	$0, \frac{1}{2}, \bar{z}$	$\frac{1}{2}, 0, \bar{z}$	$hkl : h + k = 2n$
4 g 4 . .	$0, 0, z$	$0, 0, \bar{z}$	$\frac{1}{2}, \frac{1}{2}, \bar{z}$	$\frac{1}{2}, \frac{1}{2}, z$	$hkl : h + k = 2n$
4 f . . 2/m	$\frac{1}{4}, \frac{1}{4}, \frac{1}{2}$	$\frac{3}{4}, \frac{3}{4}, \frac{1}{2}$	$\frac{3}{4}, \frac{1}{4}, \frac{1}{2}$	$\frac{1}{4}, \frac{3}{4}, \frac{1}{2}$	$hkl : h, k = 2n$
4 e . . 2/m	$\frac{1}{4}, \frac{1}{4}, 0$	$\frac{3}{4}, \frac{3}{4}, 0$	$\frac{3}{4}, \frac{1}{4}, 0$	$\frac{1}{4}, \frac{3}{4}, 0$	$hkl : h, k = 2n$
2 d $\bar{4}2m$	$0, \frac{1}{2}, \frac{1}{2}$	$\frac{1}{2}, 0, \frac{1}{2}$			$hkl : h + k = 2n$
2 c $\bar{4}2m$	$0, \frac{1}{2}, 0$	$\frac{1}{2}, 0, 0$			$hkl : h + k = 2n$
2 b 422	$0, 0, \frac{1}{2}$	$\frac{1}{2}, \frac{1}{2}, \frac{1}{2}$			$hkl : h + k = 2n$
2 a 422	$0, 0, 0$	$\frac{1}{2}, \frac{1}{2}, 0$			$hkl : h + k = 2n$

Symmetry of special projections

Along [001] $p4mm$

$$\mathbf{a}' = \frac{1}{2}(\mathbf{a} - \mathbf{b}) \quad \mathbf{b}' = \frac{1}{2}(\mathbf{a} + \mathbf{b})$$

Origin at 0, 0, z

Along [100] $p2mm$

$$\mathbf{a}' = \frac{1}{2}\mathbf{b} \quad \mathbf{b}' = \mathbf{c}$$

Origin at x, 0, 0

Along [110] $p2mm$

$$\mathbf{a}' = \frac{1}{2}(-\mathbf{a} + \mathbf{b}) \quad \mathbf{b}' = \mathbf{c}$$

Origin at x, x, 0

Maximal non-isomorphic subgroups

I	[2] $P\bar{4}b2$ (117)	1; 2; 7; 8; 11; 12; 13; 14
	[2] $P\bar{4}2m$ (111)	1; 2; 5; 6; 11; 12; 15; 16
	[2] $P4bm$ (100)	1; 2; 3; 4; 13; 14; 15; 16
	[2] $P422$ (89)	1; 2; 3; 4; 5; 6; 7; 8
	[2] $P4/n11$ ($P4/n$, 85)	1; 2; 3; 4; 9; 10; 11; 12
	[2] $P2/n12/m$ ($Cmme$, 67)	1; 2; 7; 8; 9; 10; 15; 16
	[2] $P2/n2/b1$ ($Pban$, 50)	1; 2; 5; 6; 9; 10; 13; 14

IIa none

IIIb [2] $P4_2/nm$ ($c' = 2c$) (134); [2] $P4_2/nbc$ ($c' = 2c$) (133); [2] $P4/nnc$ ($c' = 2c$) (126)

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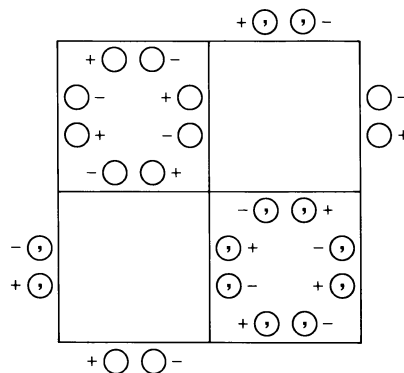
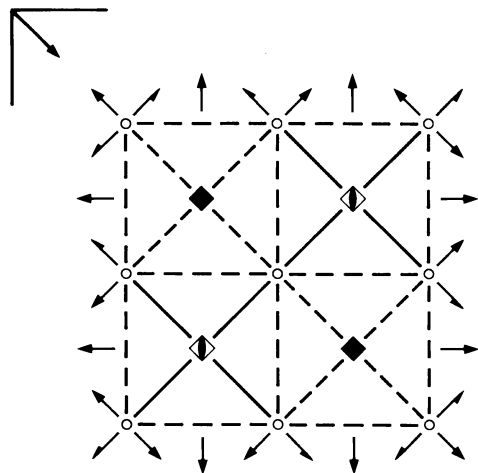
$P4/nbm$ D_{4h}^3 $4/mmm$

Tetragonal

No. 125

 $P 4/n 2/b 2/m$ Patterson symmetry $P4/mmm$

ORIGIN CHOICE 2

**Origin** at centre $(2/m)$ at $n(b, a)(2, 1/g, 2/m)$, at $\frac{1}{4}, \frac{1}{4}, 0$ from 422**Asymmetric unit** $-\frac{1}{4} \leq x \leq \frac{1}{4}; -\frac{1}{4} \leq y \leq \frac{1}{4}; 0 \leq z \leq \frac{1}{2}; x \leq -y$ **Symmetry operations**

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

Maximal isomorphic subgroups of lowest index**IIc** [2] $P4/nbm$ ($c' = 2c$) (125); [9] $P4/nbm$ ($a' = 3a, b' = 3b$) (125)**Minimal non-isomorphic supergroups****I** none**II** [2] $C4/mmm$ ($P4/mmm$, 123); [2] $I4/mcm$ (140)

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>n</i> 1	(1) x, y, z (2) $\bar{x} + \frac{1}{2}, \bar{y} + \frac{1}{2}, z$ (3) $\bar{y} + \frac{1}{2}, x, z$ (4) $y, \bar{x} + \frac{1}{2}, z$ (5) $\bar{x} + \frac{1}{2}, y, \bar{z}$ (6) $x, \bar{y} + \frac{1}{2}, \bar{z}$ (7) y, x, \bar{z} (8) $\bar{y} + \frac{1}{2}, \bar{x} + \frac{1}{2}, \bar{z}$ (9) $\bar{x}, \bar{y}, \bar{z}$ (10) $x + \frac{1}{2}, y + \frac{1}{2}, \bar{z}$ (11) $y + \frac{1}{2}, \bar{x}, \bar{z}$ (12) $\bar{y}, x + \frac{1}{2}, \bar{z}$ (13) $x + \frac{1}{2}, \bar{y}, z$ (14) $\bar{x}, y + \frac{1}{2}, z$ (15) \bar{y}, \bar{x}, z (16) $y + \frac{1}{2}, x + \frac{1}{2}, z$	$hk0 : h + k = 2n$ $0kl : k = 2n$ $h00 : h = 2n$
		Special: as above, plus
8 <i>m</i> .. <i>m</i>	x, \bar{x}, z $\bar{x} + \frac{1}{2}, \bar{x}, \bar{z}$ $\bar{x} + \frac{1}{2}, x + \frac{1}{2}, z$ $x, x + \frac{1}{2}, \bar{z}$ $x + \frac{1}{2}, x, z$ \bar{x}, x, \bar{z} $\bar{x}, \bar{x} + \frac{1}{2}, z$ $x + \frac{1}{2}, \bar{x} + \frac{1}{2}, \bar{z}$	no extra conditions
8 <i>l</i> .2.	$x, \frac{1}{4}, \frac{1}{2}$ $\bar{x}, \frac{3}{4}, \frac{1}{2}$ $\bar{x} + \frac{1}{2}, \frac{1}{4}, \frac{1}{2}$ $x + \frac{1}{2}, \frac{3}{4}, \frac{1}{2}$ $\frac{1}{4}, x, \frac{1}{2}$ $\frac{3}{4}, \bar{x}, \frac{1}{2}$ $\frac{1}{4}, \bar{x} + \frac{1}{2}, \frac{1}{2}$ $\frac{3}{4}, x + \frac{1}{2}, \frac{1}{2}$	$hkl : h + k = 2n$
8 <i>k</i> .2.	$x, \frac{1}{4}, 0$ $\bar{x}, \frac{3}{4}, 0$ $\bar{x} + \frac{1}{2}, \frac{1}{4}, 0$ $x + \frac{1}{2}, \frac{3}{4}, 0$ $\frac{1}{4}, x, 0$ $\frac{3}{4}, \bar{x}, 0$ $\frac{1}{4}, \bar{x} + \frac{1}{2}, 0$ $\frac{3}{4}, x + \frac{1}{2}, 0$	$hkl : h + k = 2n$
8 <i>j</i> ..2	$x, x, \frac{1}{2}$ $\bar{x}, \bar{x}, \frac{1}{2}$ $\bar{x} + \frac{1}{2}, \bar{x} + \frac{1}{2}, \frac{1}{2}$ $x + \frac{1}{2}, x + \frac{1}{2}, \frac{1}{2}$ $\bar{x} + \frac{1}{2}, x, \frac{1}{2}$ $x + \frac{1}{2}, \bar{x}, \frac{1}{2}$ $x, \bar{x} + \frac{1}{2}, \frac{1}{2}$ $\bar{x}, x + \frac{1}{2}, \frac{1}{2}$	$hkl : h + k = 2n$
8 <i>i</i> ..2	$x, x, 0$ $\bar{x}, \bar{x}, 0$ $\bar{x} + \frac{1}{2}, \bar{x} + \frac{1}{2}, 0$ $x + \frac{1}{2}, x + \frac{1}{2}, 0$ $\bar{x} + \frac{1}{2}, x, 0$ $x + \frac{1}{2}, \bar{x}, 0$ $x, \bar{x} + \frac{1}{2}, 0$ $\bar{x}, x + \frac{1}{2}, 0$	$hkl : h + k = 2n$
4 <i>h</i> 2.. <i>mm</i>	$\frac{3}{4}, \frac{1}{4}, z$ $\frac{1}{4}, \frac{3}{4}, z$ $\frac{1}{4}, \frac{3}{4}, \bar{z}$ $\frac{3}{4}, \frac{1}{4}, \bar{z}$ $\frac{3}{4}, \frac{1}{4}, z$ $\frac{1}{4}, \frac{3}{4}, \bar{z}$ $\frac{3}{4}, \frac{3}{4}, z$ $\frac{1}{4}, \frac{1}{4}, z$ $\frac{1}{4}, \frac{1}{4}, \bar{z}$ $\frac{3}{4}, \frac{3}{4}, \bar{z}$ $\frac{3}{4}, \frac{3}{4}, z$	$hkl : h + k = 2n$
4 <i>g</i> 4..	$\frac{1}{4}, \frac{1}{4}, z$ $\frac{1}{4}, \frac{1}{4}, \bar{z}$ $\frac{3}{4}, \frac{3}{4}, \bar{z}$ $\frac{3}{4}, \frac{3}{4}, z$	$hkl : h + k = 2n$
4 <i>f</i> ..2/ <i>m</i>	$0, 0, \frac{1}{2}$ $\frac{1}{2}, \frac{1}{2}, \frac{1}{2}$ $\frac{1}{2}, 0, \frac{1}{2}$ $0, \frac{1}{2}, \frac{1}{2}$	$hkl : h, k = 2n$
4 <i>e</i> ..2/ <i>m</i>	$0, 0, 0$ $\frac{1}{2}, \frac{1}{2}, 0$ $\frac{1}{2}, 0, 0$ $0, \frac{1}{2}, 0$	$hkl : h, k = 2n$
2 <i>d</i> $\bar{4}2m$	$\frac{3}{4}, \frac{1}{4}, \frac{1}{2}$ $\frac{1}{4}, \frac{3}{4}, \frac{1}{2}$	$hkl : h + k = 2n$
2 <i>c</i> $\bar{4}2m$	$\frac{3}{4}, \frac{1}{4}, 0$ $\frac{1}{4}, \frac{3}{4}, 0$	$hkl : h + k = 2n$
2 <i>b</i> 422	$\frac{1}{4}, \frac{1}{4}, \frac{1}{2}$ $\frac{3}{4}, \frac{3}{4}, \frac{1}{2}$	$hkl : h + k = 2n$
2 <i>a</i> 422	$\frac{1}{4}, \frac{1}{4}, 0$ $\frac{3}{4}, \frac{3}{4}, 0$	$hkl : h + k = 2n$

Symmetry of special projectionsAlong [001] $p4mm$

$$\mathbf{a}' = \frac{1}{2}(\mathbf{a} - \mathbf{b}) \quad \mathbf{b}' = \frac{1}{2}(\mathbf{a} + \mathbf{b})$$

Origin at $\frac{1}{4}, \frac{1}{4}, z$ Along [100] $p2mm$

$$\mathbf{a}' = \frac{1}{2}\mathbf{b} \quad \mathbf{b}' = \mathbf{c}$$

Origin at $x, 0, 0$ Along [110] $p2mm$

$$\mathbf{a}' = \frac{1}{2}(-\mathbf{a} + \mathbf{b}) \quad \mathbf{b}' = \mathbf{c}$$

Origin at $x, x, 0$ **Maximal non-isomorphic subgroups**

I	[2] $P\bar{4}b2$ (117)	1; 2; 7; 8; 11; 12; 13; 14
	[2] $P\bar{4}2m$ (111)	1; 2; 5; 6; 11; 12; 15; 16
	[2] $P4bm$ (100)	1; 2; 3; 4; 13; 14; 15; 16
	[2] $P422$ (89)	1; 2; 3; 4; 5; 6; 7; 8
	[2] $P4/n11$ ($P4/n$, 85)	1; 2; 3; 4; 9; 10; 11; 12
	[2] $P2/n12/m$ ($Cmme$, 67)	1; 2; 7; 8; 9; 10; 15; 16
	[2] $P2/n2/b1$ ($Pban$, 50)	1; 2; 5; 6; 9; 10; 13; 14

IIa none**IIb** [2] $P4_2/nm$ ($\mathbf{c}' = 2\mathbf{c}$) (134); [2] $P4_2/nbc$ ($\mathbf{c}' = 2\mathbf{c}$) (133); [2] $P4/nnc$ ($\mathbf{c}' = 2\mathbf{c}$) (126)

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