

$P4/nnc$

$D_{4h}^4$

$4/mmm$

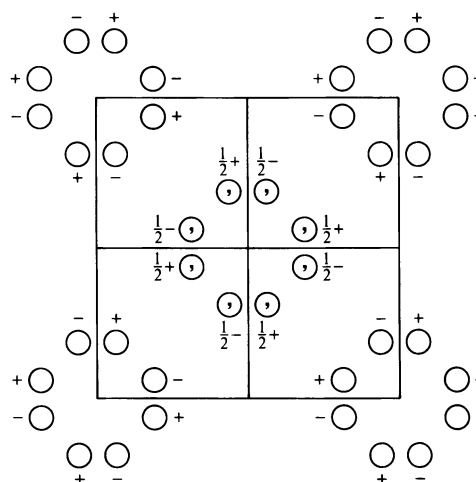
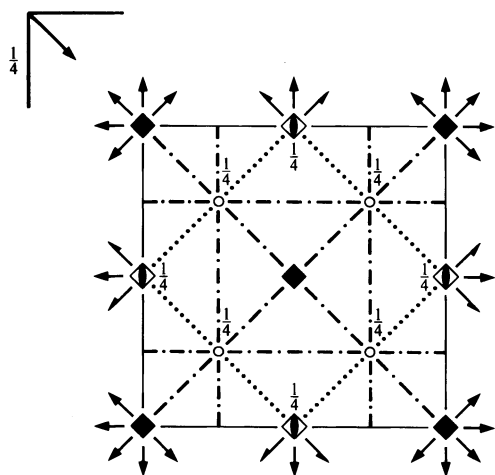
Tetragonal

No. 126

$P 4/n 2/n 2/c$

Patterson symmetry  $P4/mmm$

ORIGIN CHOICE 1



**Origin** at  $422/n$ , at  $-\frac{1}{4}, -\frac{1}{4}, -\frac{1}{4}$  from  $\bar{1}$

**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 $0, y, 0$   | (6) 2 $x, 0, 0$   | (7) 2 $x, x, 0$   | (8) 2 $x, \bar{x}, 0$   |
| (9) $\bar{1}$ $\frac{1}{4}, \frac{1}{4}, \frac{1}{4}$     | (10) $n(\frac{1}{2}, \frac{1}{2}, 0)$ $x, y, \frac{1}{4}$ | (11) $\bar{4}^+$ $\frac{1}{2}, 0, z; \frac{1}{2}, 0, \frac{1}{4}$ | (12) $\bar{4}^-$ $0, \frac{1}{2}, z; 0, \frac{1}{2}, \frac{1}{4}$ |
| (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
16 <i>k</i> 1	(1) $x, y, z$ (5) $\bar{x}, y, \bar{z}$ (9) $\bar{x} + \frac{1}{2}, \bar{y} + \frac{1}{2}, \bar{z} + \frac{1}{2}$ (13) $x + \frac{1}{2}, \bar{y} + \frac{1}{2}, z + \frac{1}{2}$	(2) $\bar{x}, \bar{y}, z$ (6) $x, \bar{y}, \bar{z}$ (10) $x + \frac{1}{2}, y + \frac{1}{2}, \bar{z} + \frac{1}{2}$ (14) $\bar{x} + \frac{1}{2}, y + \frac{1}{2}, z + \frac{1}{2}$
	(3) $\bar{y}, x, z$ (7) $y, x, \bar{z}$ (11) $y + \frac{1}{2}, \bar{x} + \frac{1}{2}, \bar{z} + \frac{1}{2}$ (15) $\bar{y} + \frac{1}{2}, \bar{x} + \frac{1}{2}, z + \frac{1}{2}$	(4) $y, \bar{x}, z$ (8) $\bar{y}, \bar{x}, \bar{z}$ (12) $\bar{y} + \frac{1}{2}, x + \frac{1}{2}, \bar{z} + \frac{1}{2}$ (16) $y + \frac{1}{2}, x + \frac{1}{2}, z + \frac{1}{2}$
		General: $hk0 : h + k = 2n$ $0kl : k + l = 2n$ $hhl : l = 2n$ $00l : l = 2n$ $h00 : h = 2n$
		Special: as above, plus
8 <i>j</i> .2.	$x, 0, \frac{1}{2}$ $\bar{x} + \frac{1}{2}, \frac{1}{2}, 0$	$\bar{x}, 0, \frac{1}{2}$ $x + \frac{1}{2}, \frac{1}{2}, 0$
	$0, x, \frac{1}{2}$ $\frac{1}{2}, \bar{x} + \frac{1}{2}, 0$	$0, \bar{x}, \frac{1}{2}$ $\frac{1}{2}, x + \frac{1}{2}, 0$
8 <i>i</i> .2.	$x, 0, 0$ $\bar{x} + \frac{1}{2}, \frac{1}{2}, \frac{1}{2}$	$\bar{x}, 0, 0$ $x + \frac{1}{2}, \frac{1}{2}, \frac{1}{2}$
	$0, x, 0$ $\frac{1}{2}, \bar{x} + \frac{1}{2}, \frac{1}{2}$	$0, \bar{x}, 0$ $\frac{1}{2}, x + \frac{1}{2}, \frac{1}{2}$
8 <i>h</i> ..2	$x, x, 0$ $\bar{x} + \frac{1}{2}, \bar{x} + \frac{1}{2}, \frac{1}{2}$	$\bar{x}, \bar{x}, 0$ $x + \frac{1}{2}, x + \frac{1}{2}, \frac{1}{2}$
	$\bar{x}, x, 0$ $x + \frac{1}{2}, \bar{x} + \frac{1}{2}, \frac{1}{2}$	$x, \bar{x}, 0$ $\bar{x} + \frac{1}{2}, x + \frac{1}{2}, \frac{1}{2}$
8 <i>g</i> 2..	$\frac{1}{2}, 0, z$ $0, \frac{1}{2}, \bar{z} + \frac{1}{2}$	$0, \frac{1}{2}, z$ $\frac{1}{2}, 0, \bar{z} + \frac{1}{2}$
	$\frac{1}{2}, 0, \bar{z}$ $0, \frac{1}{2}, z + \frac{1}{2}$	$0, \frac{1}{2}, \bar{z}$ $\frac{1}{2}, 0, z + \frac{1}{2}$
8 <i>f</i> $\bar{1}$	$\frac{1}{4}, \frac{1}{4}, \frac{1}{4}$ $\frac{3}{4}, \frac{3}{4}, \frac{1}{4}$	$\frac{3}{4}, \frac{1}{4}, \frac{1}{4}$ $\frac{1}{4}, \frac{3}{4}, \frac{1}{4}$
	$\frac{1}{4}, \frac{3}{4}, \frac{1}{4}$ $\frac{3}{4}, \frac{1}{4}, \frac{3}{4}$	$\frac{1}{4}, \frac{3}{4}, \frac{3}{4}$ $\frac{3}{4}, \frac{1}{4}, \frac{3}{4}$
4 <i>e</i> 4..	$0, 0, z$ $0, 0, \bar{z}$	$\frac{1}{2}, \frac{1}{2}, \bar{z} + \frac{1}{2}$ $\frac{1}{2}, \frac{1}{2}, z + \frac{1}{2}$
4 <i>d</i> $\bar{4}$ ..	$\frac{1}{2}, 0, \frac{1}{4}$ $0, \frac{1}{2}, \frac{1}{4}$	$\frac{1}{2}, 0, \frac{3}{4}$ $0, \frac{1}{2}, \frac{3}{4}$
4 <i>c</i> 222.	$\frac{1}{2}, 0, 0$ $0, \frac{1}{2}, 0$	$0, \frac{1}{2}, \frac{1}{2}$ $\frac{1}{2}, 0, \frac{1}{2}$
2 <i>b</i> 422	$0, 0, \frac{1}{2}$ $\frac{1}{2}, \frac{1}{2}, 0$	
2 <i>a</i> 422	$0, 0, 0$ $\frac{1}{2}, \frac{1}{2}, \frac{1}{2}$	

**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]  $c2mm$

$$\mathbf{a}' = \mathbf{b} \quad \mathbf{b}' = \mathbf{c}$$

Origin at x, 0, 0

Along [110]  $p2mm$

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

Origin at x, x, 0

**Maximal non-isomorphic subgroups**

<b>I</b>	[2] $P\bar{4}n2$ (118)	1; 2; 7; 8; 11; 12; 13; 14
	[2] $P\bar{4}2c$ (112)	1; 2; 5; 6; 11; 12; 15; 16
	[2] $P4nc$ (104)	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] $P2/n12/c$ ( $Ccce$ , 68)	1; 2; 7; 8; 9; 10; 15; 16
	[2] $P2/n2/n1$ ( $Pnnn$ , 48)	1; 2; 5; 6; 9; 10; 13; 14

**IIa** none

**IIb** none

**Maximal isomorphic subgroups of lowest index**

**IIc** [3]  $P4/nnc$  ( $\mathbf{c}' = 3\mathbf{c}$ ) (126); [9]  $P4/nnc$  ( $\mathbf{a}' = 3\mathbf{a}, \mathbf{b}' = 3\mathbf{b}$ ) (126)

**Minimal non-isomorphic supergroups**

**I** [3]  $Pn\bar{3}n$  (222)

**II** [2]  $I4/mmm$  (139); [2]  $C4/mcc$  ( $P4/mcc$ , 124); [2]  $P4/nbm$  ( $\mathbf{c}' = \frac{1}{2}\mathbf{c}$ ) (125)

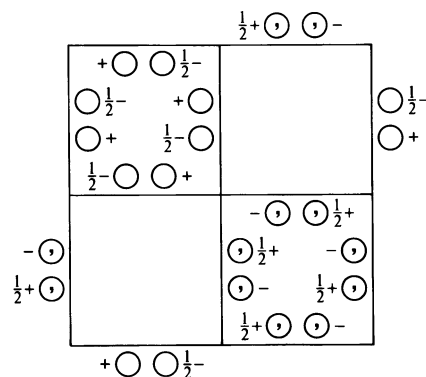
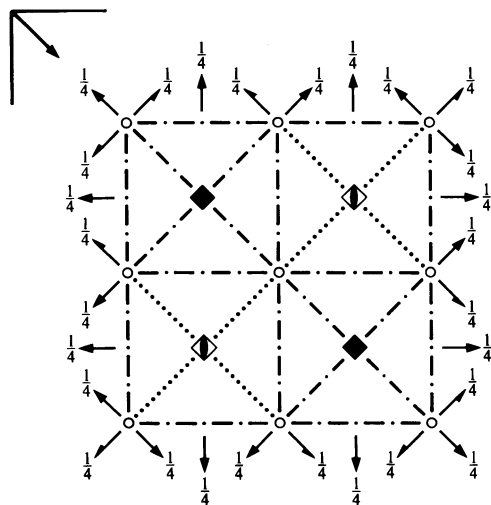
$P4/nnc$  $D_{4h}^4$  $4/mmm$ 

Tetragonal

No. 126

 $P 4/n 2/n 2/c$ Patterson symmetry  $P4/mmm$ 

ORIGIN CHOICE 2

**Origin** at  $\bar{1}$  at  $nn(n,c)$ , at  $\frac{1}{4}, \frac{1}{4}, \frac{1}{4}$  from 422**Asymmetric unit**  $-\frac{1}{4} \leq x \leq \frac{1}{4}; -\frac{1}{4} \leq y \leq \frac{1}{4}; 0 \leq z \leq \frac{1}{4}$ **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 $\frac{1}{4}, y, \frac{1}{4}$             | (6) 2 $x, \frac{1}{4}, \frac{1}{4}$             | (7) 2 $x, x, \frac{1}{4}$   | (8) 2 $x, \bar{x} + \frac{1}{2}, \frac{1}{4}$                                 |
| (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) $n(\frac{1}{2}, 0, \frac{1}{2})$ $x, 0, z$ | (14) $n(0, \frac{1}{2}, \frac{1}{2})$ $0, y, z$ | (15) $c$ $x, \bar{x}, z$  | (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
16 <i>k</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) $\bar{x} + \frac{1}{2}, y, \bar{z} + \frac{1}{2}$ (6) $x, \bar{y} + \frac{1}{2}, \bar{z} + \frac{1}{2}$ (7) $y, x, \bar{z} + \frac{1}{2}$ (8) $\bar{y} + \frac{1}{2}, \bar{x} + \frac{1}{2}, \bar{z} + \frac{1}{2}$ (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) $x + \frac{1}{2}, \bar{y}, z + \frac{1}{2}$ (14) $\bar{x}, y + \frac{1}{2}, z + \frac{1}{2}$ (15) $\bar{y}, \bar{x}, z + \frac{1}{2}$ (16) $y + \frac{1}{2}, x + \frac{1}{2}, z + \frac{1}{2}$	General: $hk0 : h + k = 2n$ $0kl : k + l = 2n$ $hhl : l = 2n$ $00l : l = 2n$ $h00 : h = 2n$  Special: as above, plus
8 <i>j</i> .2.	$x, \frac{3}{4}, \frac{1}{4}$ $\bar{x} + \frac{1}{2}, \frac{3}{4}, \frac{1}{4}$ $\frac{3}{4}, x, \frac{1}{4}$ $\frac{3}{4}, \bar{x} + \frac{1}{2}, \frac{1}{4}$ $\bar{x}, \frac{3}{4}, \frac{3}{4}$ $x + \frac{1}{2}, \frac{3}{4}, \frac{3}{4}$ $\frac{1}{4}, \bar{x}, \frac{3}{4}$ $\frac{1}{4}, x + \frac{1}{2}, \frac{3}{4}$	$hkl : h + k + l = 2n$
8 <i>i</i> .2.	$x, \frac{1}{4}, \frac{1}{4}$ $\bar{x} + \frac{1}{2}, \frac{1}{4}, \frac{1}{4}$ $\frac{1}{4}, x, \frac{1}{4}$ $\frac{1}{4}, \bar{x} + \frac{1}{2}, \frac{1}{4}$ $\bar{x}, \frac{3}{4}, \frac{3}{4}$ $x + \frac{1}{2}, \frac{3}{4}, \frac{3}{4}$ $\frac{3}{4}, \bar{x}, \frac{3}{4}$ $\frac{3}{4}, x + \frac{1}{2}, \frac{3}{4}$	$hkl : h + k + l = 2n$
8 <i>h</i> ..2	$x, x, \frac{1}{4}$ $\bar{x} + \frac{1}{2}, \bar{x} + \frac{1}{2}, \frac{1}{4}$ $\bar{x} + \frac{1}{2}, x, \frac{1}{4}$ $x, \bar{x} + \frac{1}{2}, \frac{1}{4}$ $\bar{x}, \bar{x}, \frac{3}{4}$ $x + \frac{1}{2}, x + \frac{1}{2}, \frac{3}{4}$ $x + \frac{1}{2}, \bar{x}, \frac{3}{4}$ $\bar{x}, x + \frac{1}{2}, \frac{3}{4}$	$hkl : h + k + l = 2n$
8 <i>g</i> 2..	$\frac{1}{4}, \frac{3}{4}, z$ $\frac{3}{4}, \frac{1}{4}, z$ $\frac{1}{4}, \frac{3}{4}, \bar{z} + \frac{1}{2}$ $\frac{3}{4}, \frac{1}{4}, \bar{z} + \frac{1}{2}$ $\frac{3}{4}, \frac{1}{4}, \bar{z}$ $\frac{1}{4}, \frac{3}{4}, \bar{z}$ $\frac{3}{4}, \frac{1}{4}, z + \frac{1}{2}$ $\frac{1}{4}, \frac{3}{4}, z + \frac{1}{2}$	$hkl : h + k, l = 2n$
8 <i>f</i> $\bar{1}$	0,0,0 $\frac{1}{2}, \frac{1}{2}, 0$ $\frac{1}{2}, 0, 0$ 0, $\frac{1}{2}, 0$ $\frac{1}{2}, 0, \frac{1}{2}$ 0, $\frac{1}{2}, \frac{1}{2}$ 0, 0, $\frac{1}{2}$ $\frac{1}{2}, \frac{1}{2}, \frac{1}{2}$	$hkl : h, k, l = 2n$
4 <i>e</i> 4..	$\frac{1}{4}, \frac{1}{4}, z$ $\frac{1}{4}, \frac{1}{4}, \bar{z} + \frac{1}{2}$ $\frac{3}{4}, \frac{3}{4}, \bar{z}$ $\frac{3}{4}, \frac{3}{4}, z + \frac{1}{2}$	$hkl : h + k + l = 2n$
4 <i>d</i> $\bar{4}$ ..	$\frac{1}{4}, \frac{3}{4}, 0$ $\frac{3}{4}, \frac{1}{4}, 0$ $\frac{1}{4}, \frac{3}{4}, \frac{1}{2}$ $\frac{3}{4}, \frac{1}{4}, \frac{1}{2}$	$hkl : h + k, l = 2n$
4 <i>c</i> 222.	$\frac{1}{4}, \frac{3}{4}, \frac{3}{4}$ $\frac{3}{4}, \frac{1}{4}, \frac{3}{4}$ $\frac{3}{4}, \frac{1}{4}, \frac{1}{4}$ $\frac{1}{4}, \frac{3}{4}, \frac{1}{4}$	$hkl : h + k, l = 2n$
2 <i>b</i> 422	$\frac{1}{4}, \frac{1}{4}, \frac{3}{4}$ $\frac{3}{4}, \frac{3}{4}, \frac{1}{4}$	$hkl : h + k + l = 2n$
2 <i>a</i> 422	$\frac{1}{4}, \frac{1}{4}, \frac{1}{4}$ $\frac{3}{4}, \frac{3}{4}, \frac{3}{4}$	$hkl : h + k + l = 2n$

**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  $\frac{1}{4}, \frac{1}{4}, z$

Along [100]  $c2mm$

$$\mathbf{a}' = \mathbf{b} \quad \mathbf{b}' = \mathbf{c}$$

Origin at  $x, \frac{1}{4}, \frac{1}{4}$

Along [110]  $p2mm$

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

Origin at  $x, x, 0$

**Maximal non-isomorphic subgroups**

<b>I</b>	[2] $P\bar{4}n2$ (118)	1; 2; 7; 8; 11; 12; 13; 14
	[2] $P\bar{4}2c$ (112)	1; 2; 5; 6; 11; 12; 15; 16
	[2] $P4nc$ (104)	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] $P2/n12/c$ ( $Ccce$ , 68)	1; 2; 7; 8; 9; 10; 15; 16
	[2] $P2/n2/n1$ ( $Pnnn$ , 48)	1; 2; 5; 6; 9; 10; 13; 14

**IIa** none

**IIb** none

**Maximal isomorphic subgroups of lowest index**

**IIc** [3]  $P4/nnc$  ( $c' = 3c$ ) (126); [9]  $P4/nnc$  ( $\mathbf{a}' = 3\mathbf{a}, \mathbf{b}' = 3\mathbf{b}$ ) (126)

**Minimal non-isomorphic supergroups**

**I** [3]  $Pn\bar{3}n$  (222)

**II** [2]  $I4/mmm$  (139); [2]  $C4/mcc$  ( $P4/mcc$ , 124); [2]  $P4/nbm$  ( $\mathbf{c}' = \frac{1}{2}\mathbf{c}$ ) (125)