

$P4/nnc$

D_{4h}^4

$4/mmm$

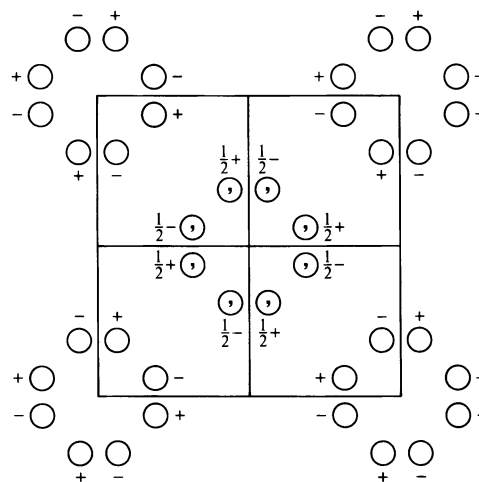
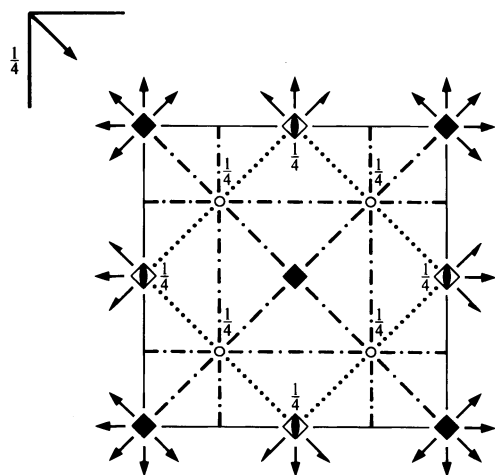
Tetragonal

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			
						General:			
16	k 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) $y + \frac{1}{2}, x + \frac{1}{2}, z + \frac{1}{2}$	$hk0: h + k = 2n$ $0kl: k + l = 2n$ $hhl: l = 2n$ $00l: l = 2n$ $h00: h = 2n$			
						Special: as above, plus			
8	j .2.	$x, 0, \frac{1}{2}$ $\bar{x} + \frac{1}{2}, \frac{1}{2}, 0$	$\bar{x}, 0, \frac{1}{2}$ $x + \frac{1}{2}, \frac{1}{2}, 0$	$0, x, \frac{1}{2}$ $\frac{1}{2}, \bar{x} + \frac{1}{2}, 0$	$0, \bar{x}, \frac{1}{2}$ $\frac{1}{2}, x + \frac{1}{2}, 0$	$hkl: h + k + l = 2n$			
8	i .2.	$x, 0, 0$ $\bar{x} + \frac{1}{2}, \frac{1}{2}, \frac{1}{2}$	$\bar{x}, 0, 0$ $x + \frac{1}{2}, \frac{1}{2}, \frac{1}{2}$	$0, x, 0$ $\frac{1}{2}, \bar{x} + \frac{1}{2}, \frac{1}{2}$	$0, \bar{x}, 0$ $\frac{1}{2}, x + \frac{1}{2}, \frac{1}{2}$	$hkl: h + k + l = 2n$			
8	h ..2	$x, x, 0$ $\bar{x} + \frac{1}{2}, \bar{x} + \frac{1}{2}, \frac{1}{2}$	$\bar{x}, \bar{x}, 0$ $x + \frac{1}{2}, x + \frac{1}{2}, \frac{1}{2}$	$\bar{x}, x, 0$ $x + \frac{1}{2}, \bar{x} + \frac{1}{2}, \frac{1}{2}$	$x, \bar{x}, 0$ $\bar{x} + \frac{1}{2}, x + \frac{1}{2}, \frac{1}{2}$	$hkl: h + k + l = 2n$			
8	g 2..	$\frac{1}{2}, 0, z$ $0, \frac{1}{2}, \bar{z} + \frac{1}{2}$	$0, \frac{1}{2}, z$ $\frac{1}{2}, 0, \bar{z} + \frac{1}{2}$	$\frac{1}{2}, 0, \bar{z}$ $0, \frac{1}{2}, z + \frac{1}{2}$	$0, \frac{1}{2}, \bar{z}$ $\frac{1}{2}, 0, z + \frac{1}{2}$	$hkl: h + k, l = 2n$			
8	f $\bar{1}$	$\frac{1}{4}, \frac{1}{4}, \frac{1}{4}$	$\frac{3}{4}, \frac{3}{4}, \frac{1}{4}$	$\frac{3}{4}, \frac{1}{4}, \frac{1}{4}$	$\frac{1}{4}, \frac{3}{4}, \frac{1}{4}$	$\frac{3}{4}, \frac{1}{4}, \frac{3}{4}$	$\frac{1}{4}, \frac{1}{4}, \frac{3}{4}$	$\frac{3}{4}, \frac{3}{4}, \frac{3}{4}$	$hkl: h, k, l = 2n$
4	e 4..	$0, 0, z$	$0, 0, \bar{z}$	$\frac{1}{2}, \frac{1}{2}, \bar{z} + \frac{1}{2}$	$\frac{1}{2}, \frac{1}{2}, z + \frac{1}{2}$	$hkl: h + k + l = 2n$			
4	d $\bar{4}$..	$\frac{1}{2}, 0, \frac{1}{4}$	$0, \frac{1}{2}, \frac{1}{4}$	$\frac{1}{2}, 0, \frac{3}{4}$	$0, \frac{1}{2}, \frac{3}{4}$	$hkl: h + k, l = 2n$			
4	c 222.	$\frac{1}{2}, 0, 0$	$0, \frac{1}{2}, 0$	$0, \frac{1}{2}, \frac{1}{2}$	$\frac{1}{2}, 0, \frac{1}{2}$	$hkl: h + k, l = 2n$			
2	b 422	$0, 0, \frac{1}{2}$	$\frac{1}{2}, \frac{1}{2}, 0$			$hkl: h + k + l = 2n$			
2	a 422	$0, 0, 0$	$\frac{1}{2}, \frac{1}{2}, \frac{1}{2}$			$hkl: h + k + l = 2n$			

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 $0, 0, z$ 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 $x, x, 0$

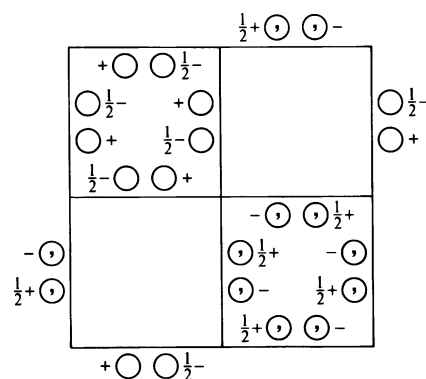
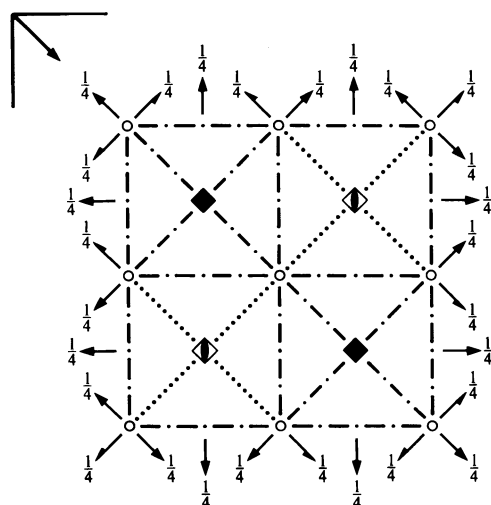
$P4/nnc$ D_{4h}^4 $4/mmm$

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 422Asymmetric 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				
General:										
16	<i>k</i> 1	(1) x, y, z (5) $\bar{x} + \frac{1}{2}, y, \bar{z} + \frac{1}{2}$ (9) $\bar{x}, \bar{y}, \bar{z}$ (13) $x + \frac{1}{2}, \bar{y}, z + \frac{1}{2}$	(2) $\bar{x} + \frac{1}{2}, \bar{y} + \frac{1}{2}, z$ (6) $x, \bar{y} + \frac{1}{2}, \bar{z} + \frac{1}{2}$ (10) $x + \frac{1}{2}, y + \frac{1}{2}, \bar{z}$ (14) $\bar{x}, y + \frac{1}{2}, z + \frac{1}{2}$	(3) $\bar{y} + \frac{1}{2}, x, z$ (7) $y, x, \bar{z} + \frac{1}{2}$ (11) $y + \frac{1}{2}, \bar{x}, \bar{z}$ (15) $\bar{y}, \bar{x}, z + \frac{1}{2}$	(4) $y, \bar{x} + \frac{1}{2}, z$ (8) $\bar{y} + \frac{1}{2}, \bar{x} + \frac{1}{2}, \bar{z} + \frac{1}{2}$ (12) $\bar{y}, x + \frac{1}{2}, \bar{z}$ (16) $y + \frac{1}{2}, x + \frac{1}{2}, z + \frac{1}{2}$	$hk0: h + k = 2n$ $0kl: k + l = 2n$ $hhl: l = 2n$ $00l: l = 2n$ $h00: h = 2n$				
Special: as above, plus										
8	<i>j</i> .2.	$x, \frac{3}{4}, \frac{1}{4}$ $\bar{x}, \frac{1}{4}, \frac{3}{4}$	$\bar{x} + \frac{1}{2}, \frac{3}{4}, \frac{1}{4}$ $x + \frac{1}{2}, \frac{1}{4}, \frac{3}{4}$	$\frac{3}{4}, x, \frac{1}{4}$ $\frac{1}{4}, \bar{x}, \frac{3}{4}$	$\frac{3}{4}, \bar{x} + \frac{1}{2}, \frac{1}{4}$ $\frac{1}{4}, x + \frac{1}{2}, \frac{3}{4}$	$hkl: h + k + l = 2n$				
8	<i>i</i> .2.	$x, \frac{1}{4}, \frac{1}{4}$ $\bar{x}, \frac{3}{4}, \frac{3}{4}$	$\bar{x} + \frac{1}{2}, \frac{1}{4}, \frac{1}{4}$ $x + \frac{1}{2}, \frac{3}{4}, \frac{3}{4}$	$\frac{1}{4}, x, \frac{1}{4}$ $\frac{3}{4}, \bar{x}, \frac{3}{4}$	$\frac{1}{4}, \bar{x} + \frac{1}{2}, \frac{1}{4}$ $\frac{3}{4}, x + \frac{1}{2}, \frac{3}{4}$	$hkl: h + k + l = 2n$				
8	<i>h</i> ..2	$x, x, \frac{1}{4}$ $\bar{x}, \bar{x}, \frac{3}{4}$	$\bar{x} + \frac{1}{2}, \bar{x} + \frac{1}{2}, \frac{1}{4}$ $x + \frac{1}{2}, x + \frac{1}{2}, \frac{3}{4}$	$\bar{x} + \frac{1}{2}, x, \frac{1}{4}$ $x + \frac{1}{2}, \bar{x}, \frac{3}{4}$	$x, \bar{x} + \frac{1}{2}, \frac{1}{4}$ $\bar{x}, x + \frac{1}{2}, \frac{3}{4}$	$hkl: h + k + l = 2n$				
8	<i>g</i> 2..	$\frac{1}{4}, \frac{3}{4}, z$ $\frac{3}{4}, \frac{1}{4}, \bar{z}$	$\frac{3}{4}, \frac{1}{4}, z$ $\frac{1}{4}, \frac{3}{4}, \bar{z}$	$\frac{1}{4}, \frac{3}{4}, \bar{z} + \frac{1}{2}$ $\frac{3}{4}, \frac{1}{4}, z + \frac{1}{2}$	$\frac{3}{4}, \frac{1}{4}, \bar{z} + \frac{1}{2}$ $\frac{1}{4}, \frac{3}{4}, z + \frac{1}{2}$	$hkl: h + k, l = 2n$				
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 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] $c2mm$

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

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 $x, x, 0$