

$P4_2/nnm$

D_{4h}^{12}

$4/mmm$

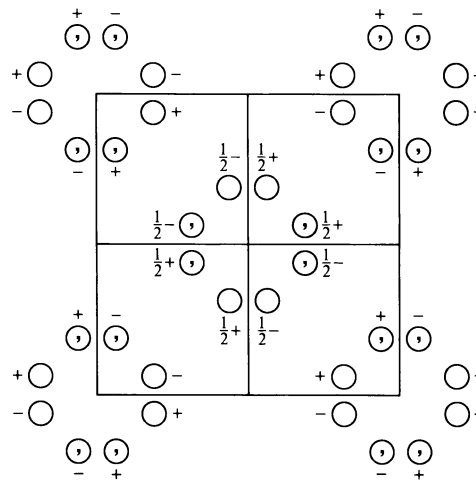
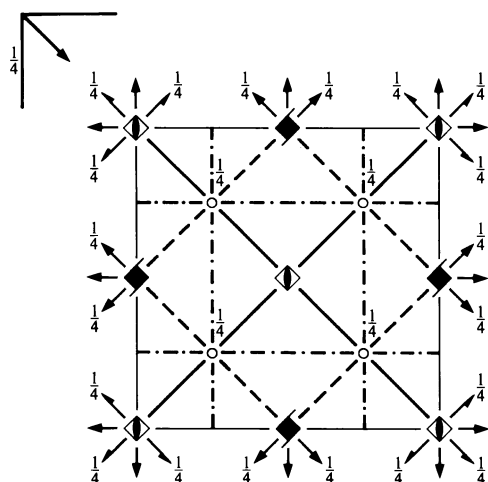
Tetragonal

No. 134

$P 4_2/n 2/n 2/m$

Patterson symmetry $P4/mmm$

ORIGIN CHOICE 1



Origin at $\bar{4}2m$, at $-\frac{1}{4}, \frac{1}{4}, -\frac{1}{4}$ from centre ($2/m$)

Asymmetric unit $0 \leq x \leq \frac{1}{2}; 0 \leq y \leq 1; 0 \leq z \leq \frac{1}{4}; x \leq y; y \leq 1-x$

Symmetry operations

- | | | | |
|---|---|--|--|
| (1) 1 | (2) 2 $0, 0, z$ | (3) $4^+(0, 0, \frac{1}{2})$ $0, \frac{1}{2}, z$ | (4) $4^-(0, 0, \frac{1}{2})$ $\frac{1}{2}, 0, z$ |
| (5) 2 $0, y, 0$ | (6) 2 $x, 0, 0$ | (7) $2(\frac{1}{2}, \frac{1}{2}, 0)$ $x, x, \frac{1}{4}$ | (8) 2 $x, \bar{x} + \frac{1}{2}, \frac{1}{4}$ |
| (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) $\bar{4}^+ 0, 0, z; 0, 0, 0$ | (12) $\bar{4}^- 0, 0, z; 0, 0, 0$ |
| (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) $m x, \bar{x}, z$ | (16) $m x, x, z$ |

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	n 1	(1) x, y, z (5) \bar{x}, y, \bar{z} (9) $\bar{x} + \frac{1}{2}, \bar{y} + \frac{1}{2}, \bar{z} + \frac{1}{2}$ (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) $\bar{y} + \frac{1}{2}, x + \frac{1}{2}, z + \frac{1}{2}$ (7) $y + \frac{1}{2}, x + \frac{1}{2}, \bar{z} + \frac{1}{2}$ (11) y, \bar{x}, \bar{z} (15) \bar{y}, \bar{x}, z	(4) $y + \frac{1}{2}, \bar{x} + \frac{1}{2}, z + \frac{1}{2}$ (8) $\bar{y} + \frac{1}{2}, \bar{x} + \frac{1}{2}, \bar{z} + \frac{1}{2}$ (12) \bar{y}, x, \bar{z} (16) y, x, z	$hk0: h+k=2n$ $0kl: k+l=2n$ $00l: l=2n$ $h00: h=2n$
						Special: as above, plus
8	m .. m	x, x, z \bar{x}, x, \bar{z}	\bar{x}, \bar{x}, z x, \bar{x}, \bar{z}	$\bar{x} + \frac{1}{2}, x + \frac{1}{2}, z + \frac{1}{2}$ $x + \frac{1}{2}, x + \frac{1}{2}, \bar{z} + \frac{1}{2}$	$x + \frac{1}{2}, \bar{x} + \frac{1}{2}, z + \frac{1}{2}$ $\bar{x} + \frac{1}{2}, \bar{x} + \frac{1}{2}, \bar{z} + \frac{1}{2}$	no extra conditions
8	l .. 2	$x, x + \frac{1}{2}, \frac{3}{4}$ $\bar{x} + \frac{1}{2}, \bar{x}, \frac{3}{4}$	$\bar{x}, \bar{x} + \frac{1}{2}, \frac{3}{4}$ $x + \frac{1}{2}, x, \frac{3}{4}$	$\bar{x}, x + \frac{1}{2}, \frac{1}{4}$ $x + \frac{1}{2}, \bar{x}, \frac{1}{4}$	$x, \bar{x} + \frac{1}{2}, \frac{1}{4}$ $\bar{x} + \frac{1}{2}, x, \frac{1}{4}$	$hkl: h+k=2n$
8	k .. 2	$x, x + \frac{1}{2}, \frac{1}{4}$ $\bar{x} + \frac{1}{2}, \bar{x}, \frac{1}{4}$	$\bar{x}, \bar{x} + \frac{1}{2}, \frac{1}{4}$ $x + \frac{1}{2}, x, \frac{1}{4}$	$\bar{x}, x + \frac{1}{2}, \frac{3}{4}$ $x + \frac{1}{2}, \bar{x}, \frac{3}{4}$	$x, \bar{x} + \frac{1}{2}, \frac{3}{4}$ $\bar{x} + \frac{1}{2}, x, \frac{3}{4}$	$hkl: h+k=2n$
8	j . 2 .	$x, 0, \frac{1}{2}$ $\bar{x} + \frac{1}{2}, \frac{1}{2}, 0$	$\bar{x}, 0, \frac{1}{2}$ $x + \frac{1}{2}, \frac{1}{2}, 0$	$\frac{1}{2}, x + \frac{1}{2}, 0$ $0, \bar{x}, \frac{1}{2}$	$\frac{1}{2}, \bar{x} + \frac{1}{2}, 0$ $0, x, \frac{1}{2}$	$hkl: h+k+l=2n$
8	i . 2 .	$x, 0, 0$ $\bar{x} + \frac{1}{2}, \frac{1}{2}, \frac{1}{2}$	$\bar{x}, 0, 0$ $x + \frac{1}{2}, \frac{1}{2}, \frac{1}{2}$	$\frac{1}{2}, x + \frac{1}{2}, \frac{1}{2}$ $0, \bar{x}, 0$	$\frac{1}{2}, \bar{x} + \frac{1}{2}, \frac{1}{2}$ $0, x, 0$	$hkl: h+k+l=2n$
8	h 2 ..	$0, \frac{1}{2}, z$ $\frac{1}{2}, 0, \bar{z} + \frac{1}{2}$	$0, \frac{1}{2}, z + \frac{1}{2}$ $\frac{1}{2}, 0, \bar{z}$	$0, \frac{1}{2}, \bar{z}$ $\frac{1}{2}, 0, z + \frac{1}{2}$	$0, \frac{1}{2}, \bar{z} + \frac{1}{2}$ $\frac{1}{2}, 0, z$	$hkl: h+k, l=2n$
4	g 2 . mm	$0, 0, z$	$\frac{1}{2}, \frac{1}{2}, z + \frac{1}{2}$	$0, 0, \bar{z}$	$\frac{1}{2}, \frac{1}{2}, \bar{z} + \frac{1}{2}$	$hkl: h+k+l=2n$
4	f .. $2/m$	$\frac{3}{4}, \frac{3}{4}, \frac{3}{4}$	$\frac{1}{4}, \frac{1}{4}, \frac{3}{4}$	$\frac{3}{4}, \frac{1}{4}, \frac{1}{4}$	$\frac{1}{4}, \frac{3}{4}, \frac{1}{4}$	$hkl: h+k, h+l, k+l=2n$
4	e .. $2/m$	$\frac{1}{4}, \frac{1}{4}, \frac{1}{4}$	$\frac{3}{4}, \frac{3}{4}, \frac{1}{4}$	$\frac{1}{4}, \frac{3}{4}, \frac{3}{4}$	$\frac{3}{4}, \frac{1}{4}, \frac{3}{4}$	$hkl: h+k, h+l, k+l=2n$
4	d 2 . 22	$0, \frac{1}{2}, \frac{1}{4}$	$0, \frac{1}{2}, \frac{3}{4}$	$\frac{1}{2}, 0, \frac{1}{4}$	$\frac{1}{2}, 0, \frac{3}{4}$	$hkl: h+k, l=2n$
4	c 2 2 2 .	$0, \frac{1}{2}, 0$	$0, \frac{1}{2}, \frac{1}{2}$	$\frac{1}{2}, 0, \frac{1}{2}$	$\frac{1}{2}, 0, 0$	$hkl: h+k, l=2n$
2	b $\bar{4}2m$	$0, 0, \frac{1}{2}$	$\frac{1}{2}, \frac{1}{2}, 0$			$hkl: h+k+l=2n$
2	a $\bar{4}2m$	$0, 0, 0$	$\frac{1}{2}, \frac{1}{2}, \frac{1}{2}$			$hkl: h+k+l=2n$

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] $p2mm$

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

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

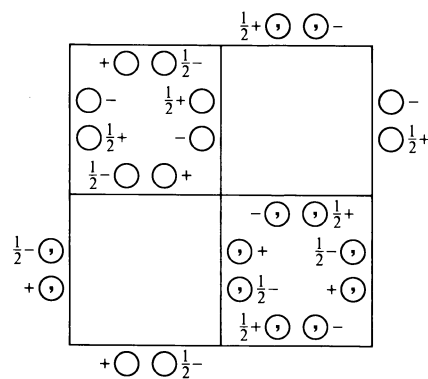
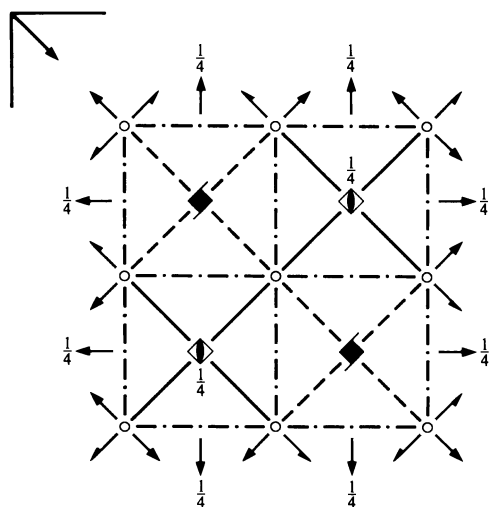
$P4_2/nnm$ D_{4h}^{12} $4/mmm$

Tetragonal

No. 134

 $P 4_2/n 2/n 2/m$ Patterson symmetry $P4/mmm$

ORIGIN CHOICE 2



Origin at centre ($2/m$) at $nn(2_1/g, 2/m)$, at $\frac{1}{4}, -\frac{1}{4}, \frac{1}{4}$ from $\bar{4}2m$

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) $4^+(0, 0, \frac{1}{2})$ $\frac{1}{4}, \frac{1}{4}, z$ | (4) $4^-(0, 0, \frac{1}{2})$ $\frac{1}{4}, \frac{1}{4}, z$ |
| (5) 2 $\frac{1}{4}, y, \frac{1}{4}$ | (6) 2 $x, \frac{1}{4}, \frac{1}{4}$ | (7) 2 $x, x, 0$ | (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) $\bar{4}^+$ $\frac{1}{4}, -\frac{1}{4}, z; \frac{1}{4}, -\frac{1}{4}, \frac{1}{4}$ | (12) $\bar{4}^-$ $-\frac{1}{4}, \frac{1}{4}, z; -\frac{1}{4}, \frac{1}{4}, \frac{1}{4}$ |
| (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) m x, \bar{x}, z | (16) $g(\frac{1}{2}, \frac{1}{2}, 0)$ 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	n 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) $\bar{y} + \frac{1}{2}, x, z + \frac{1}{2}$ (7) y, x, \bar{z} (11) $y + \frac{1}{2}, \bar{x}, \bar{z} + \frac{1}{2}$ (15) \bar{y}, \bar{x}, z	(4) $y, \bar{x} + \frac{1}{2}, z + \frac{1}{2}$ (8) $\bar{y} + \frac{1}{2}, \bar{x} + \frac{1}{2}, \bar{z}$ (12) $\bar{y}, x + \frac{1}{2}, \bar{z} + \frac{1}{2}$ (16) $y + \frac{1}{2}, x + \frac{1}{2}, z$	$hk0: h + k = 2n$ $0kl: k + l = 2n$ $00l: l = 2n$ $h00: h = 2n$
						Special: as above, plus
8	m .. m	x, \bar{x}, z $\bar{x} + \frac{1}{2}, \bar{x}, \bar{z} + \frac{1}{2}$	$\bar{x} + \frac{1}{2}, x + \frac{1}{2}, z$ $x, x + \frac{1}{2}, \bar{z} + \frac{1}{2}$	$x + \frac{1}{2}, x, z + \frac{1}{2}$ \bar{x}, x, \bar{z}	$\bar{x}, \bar{x} + \frac{1}{2}, z + \frac{1}{2}$ $x + \frac{1}{2}, \bar{x} + \frac{1}{2}, \bar{z}$	no extra conditions
8	l .. 2	$x, x, \frac{1}{2}$ $\bar{x}, \bar{x}, \frac{1}{2}$	$\bar{x} + \frac{1}{2}, \bar{x} + \frac{1}{2}, \frac{1}{2}$ $x + \frac{1}{2}, x + \frac{1}{2}, \frac{1}{2}$	$\bar{x} + \frac{1}{2}, x, 0$ $x + \frac{1}{2}, \bar{x}, 0$	$x, \bar{x} + \frac{1}{2}, 0$ $\bar{x}, x + \frac{1}{2}, 0$	$hkl: h + k = 2n$
8	k .. 2	$x, x, 0$ $\bar{x}, \bar{x}, 0$	$\bar{x} + \frac{1}{2}, \bar{x} + \frac{1}{2}, 0$ $x + \frac{1}{2}, x + \frac{1}{2}, 0$	$\bar{x} + \frac{1}{2}, x, \frac{1}{2}$ $x + \frac{1}{2}, \bar{x}, \frac{1}{2}$	$x, \bar{x} + \frac{1}{2}, \frac{1}{2}$ $\bar{x}, x + \frac{1}{2}, \frac{1}{2}$	$hkl: h + k = 2n$
8	j . 2 .	$x, \frac{1}{4}, \frac{1}{4}$ $\bar{x}, \frac{3}{4}, \frac{3}{4}$	$\bar{x} + \frac{1}{2}, \frac{1}{4}, \frac{1}{4}$ $x + \frac{1}{2}, \frac{3}{4}, \frac{3}{4}$	$\frac{1}{4}, x, \frac{3}{4}$ $\frac{3}{4}, \bar{x}, \frac{1}{4}$	$\frac{1}{4}, \bar{x} + \frac{1}{2}, \frac{3}{4}$ $\frac{3}{4}, x + \frac{1}{2}, \frac{1}{4}$	$hkl: h + k + l = 2n$
8	i . 2 .	$x, \frac{1}{4}, \frac{3}{4}$ $\bar{x}, \frac{3}{4}, \frac{1}{4}$	$\bar{x} + \frac{1}{2}, \frac{1}{4}, \frac{3}{4}$ $x + \frac{1}{2}, \frac{3}{4}, \frac{1}{4}$	$\frac{1}{4}, x, \frac{1}{4}$ $\frac{3}{4}, \bar{x}, \frac{3}{4}$	$\frac{1}{4}, \bar{x} + \frac{1}{2}, \frac{1}{4}$ $\frac{3}{4}, x + \frac{1}{2}, \frac{3}{4}$	$hkl: h + k + l = 2n$
8	h 2 ..	$\frac{1}{4}, \frac{1}{4}, z$ $\frac{3}{4}, \frac{3}{4}, \bar{z}$	$\frac{1}{4}, \frac{1}{4}, z + \frac{1}{2}$ $\frac{3}{4}, \frac{3}{4}, \bar{z} + \frac{1}{2}$	$\frac{1}{4}, \frac{1}{4}, \bar{z} + \frac{1}{2}$ $\frac{3}{4}, \frac{3}{4}, z + \frac{1}{2}$	$\frac{1}{4}, \frac{1}{4}, \bar{z}$ $\frac{3}{4}, \frac{3}{4}, z$	$hkl: h + k, l = 2n$
4	g 2 . mm	$\frac{3}{4}, \frac{1}{4}, z$	$\frac{1}{4}, \frac{3}{4}, z + \frac{1}{2}$	$\frac{3}{4}, \frac{1}{4}, \bar{z} + \frac{1}{2}$	$\frac{1}{4}, \frac{3}{4}, \bar{z}$	$hkl: h + k + l = 2n$
4	f .. 2/ m	0, 0, 0	$\frac{1}{2}, \frac{1}{2}, 0$	$\frac{1}{2}, 0, \frac{1}{2}$	$0, \frac{1}{2}, \frac{1}{2}$	$hkl: h + k, h + l, k + l = 2n$
4	e .. 2/ m	0, 0, $\frac{1}{2}$	$\frac{1}{2}, \frac{1}{2}, \frac{1}{2}$	$\frac{1}{2}, 0, 0$	$0, \frac{1}{2}, 0$	$hkl: h + k, h + l, k + l = 2n$
4	d 2 . 22	$\frac{1}{4}, \frac{1}{4}, 0$	$\frac{1}{4}, \frac{1}{4}, \frac{1}{2}$	$\frac{3}{4}, \frac{3}{4}, 0$	$\frac{3}{4}, \frac{3}{4}, \frac{1}{2}$	$hkl: h + k, l = 2n$
4	c 2 2 2 .	$\frac{1}{4}, \frac{1}{4}, \frac{1}{4}$	$\frac{1}{4}, \frac{1}{4}, \frac{3}{4}$	$\frac{3}{4}, \frac{3}{4}, \frac{3}{4}$	$\frac{3}{4}, \frac{3}{4}, \frac{1}{4}$	$hkl: h + k, l = 2n$
2	b $\bar{4}2m$	$\frac{3}{4}, \frac{1}{4}, \frac{1}{4}$	$\frac{1}{4}, \frac{3}{4}, \frac{3}{4}$			$hkl: h + k + l = 2n$
2	a $\bar{4}2m$	$\frac{1}{4}, \frac{3}{4}, \frac{1}{4}$	$\frac{3}{4}, \frac{1}{4}, \frac{3}{4}$			$hkl: h + k + l = 2n$

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] $p2mm$

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

Origin at $x, x, 0$