

$P4_2/n\bar{c}m$

D_{4h}^{16}

$4/m\bar{3}m$

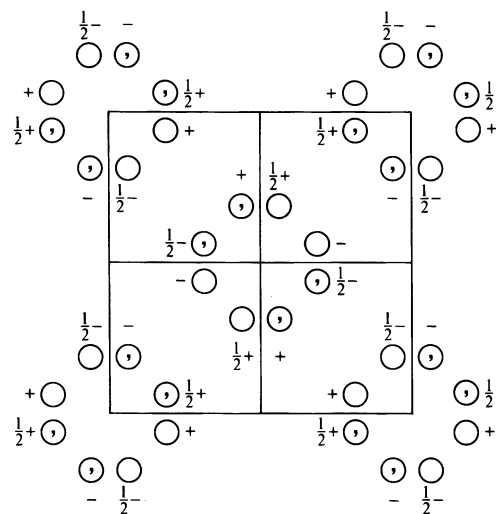
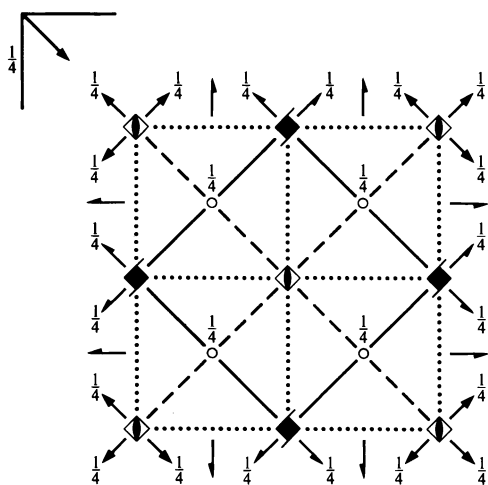
Tetragonal

No. 138

$P 4_2/n 2_1/c 2/m$

Patterson symmetry $P4/m\bar{3}m$

ORIGIN CHOICE 1



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

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

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) $2(0, \frac{1}{2}, 0)$ $\frac{1}{4}, y, 0$ | (6) $2(\frac{1}{2}, 0, 0)$ $x, \frac{1}{4}, 0$ | (7) 2 $x, x, \frac{1}{4}$ | (8) 2 $x, \bar{x}, \frac{1}{4}$ |
| (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) c $x, 0, z$ | (14) c $0, y, z$ | (15) m $x + \frac{1}{2}, \bar{x}, z$ | (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	j 1	(1) x, y, z (5) $\bar{x} + \frac{1}{2}, y + \frac{1}{2}, \bar{z}$ (9) $\bar{x} + \frac{1}{2}, \bar{y} + \frac{1}{2}, \bar{z} + \frac{1}{2}$ (13) $x, \bar{y}, z + \frac{1}{2}$	(2) \bar{x}, \bar{y}, z (6) $x + \frac{1}{2}, \bar{y} + \frac{1}{2}, \bar{z}$ (10) $x + \frac{1}{2}, y + \frac{1}{2}, \bar{z} + \frac{1}{2}$ (14) $\bar{x}, y, z + \frac{1}{2}$	(3) $\bar{y} + \frac{1}{2}, x + \frac{1}{2}, z + \frac{1}{2}$ (7) $y, x, \bar{z} + \frac{1}{2}$ (11) y, \bar{x}, \bar{z} (15) $\bar{y} + \frac{1}{2}, \bar{x} + \frac{1}{2}, z$	(4) $y + \frac{1}{2}, \bar{x} + \frac{1}{2}, z + \frac{1}{2}$ (8) $\bar{y}, \bar{x}, \bar{z} + \frac{1}{2}$ (12) \bar{y}, x, \bar{z} (16) $y + \frac{1}{2}, x + \frac{1}{2}, z$	$hk0: h+k=2n$ $0kl: l=2n$ $00l: l=2n$ $h00: h=2n$
						Special: as above, plus
8	i .. m	$x, x + \frac{1}{2}, z$ $\bar{x} + \frac{1}{2}, x, \bar{z}$	$\bar{x}, \bar{x} + \frac{1}{2}, z$ $x + \frac{1}{2}, \bar{x}, \bar{z}$	$\bar{x}, x + \frac{1}{2}, z + \frac{1}{2}$ $x + \frac{1}{2}, x, \bar{z} + \frac{1}{2}$	$x, \bar{x} + \frac{1}{2}, z + \frac{1}{2}$ $\bar{x} + \frac{1}{2}, \bar{x}, \bar{z} + \frac{1}{2}$	no extra conditions
8	h .. 2	$x, x, \frac{3}{4}$ $\bar{x} + \frac{1}{2}, \bar{x} + \frac{1}{2}, \frac{3}{4}$	$\bar{x}, \bar{x}, \frac{3}{4}$ $x + \frac{1}{2}, x + \frac{1}{2}, \frac{3}{4}$	$\bar{x} + \frac{1}{2}, x + \frac{1}{2}, \frac{1}{4}$ $x, \bar{x}, \frac{1}{4}$	$x + \frac{1}{2}, \bar{x} + \frac{1}{2}, \frac{1}{4}$ $\bar{x}, x, \frac{1}{4}$	$hkl: h+k=2n$
8	g .. 2	$x, x, \frac{1}{4}$ $\bar{x} + \frac{1}{2}, \bar{x} + \frac{1}{2}, \frac{1}{4}$	$\bar{x}, \bar{x}, \frac{1}{4}$ $x + \frac{1}{2}, x + \frac{1}{2}, \frac{1}{4}$	$\bar{x} + \frac{1}{2}, x + \frac{1}{2}, \frac{3}{4}$ $x, \bar{x}, \frac{3}{4}$	$x + \frac{1}{2}, \bar{x} + \frac{1}{2}, \frac{3}{4}$ $\bar{x}, x, \frac{3}{4}$	$hkl: h+k=2n$
8	f 2..	$0, 0, z$ $\frac{1}{2}, \frac{1}{2}, \bar{z} + \frac{1}{2}$	$\frac{1}{2}, \frac{1}{2}, z + \frac{1}{2}$ $0, 0, \bar{z}$	$\frac{1}{2}, \frac{1}{2}, \bar{z}$ $0, 0, z + \frac{1}{2}$	$0, 0, \bar{z} + \frac{1}{2}$ $\frac{1}{2}, \frac{1}{2}, z$	$hkl: h+k, l=2n$
4	e 2.. mm	$0, \frac{1}{2}, z$	$0, \frac{1}{2}, z + \frac{1}{2}$	$\frac{1}{2}, 0, \bar{z}$	$\frac{1}{2}, 0, \bar{z} + \frac{1}{2}$	$hkl: l=2n$
4	d .. $2/m$	$\frac{1}{4}, \frac{1}{4}, \frac{3}{4}$	$\frac{3}{4}, \frac{3}{4}, \frac{3}{4}$	$\frac{1}{4}, \frac{3}{4}, \frac{1}{4}$	$\frac{3}{4}, \frac{1}{4}, \frac{1}{4}$	$hkl: h+k, h+l, k+l=2n$
4	c .. $2/m$	$\frac{1}{4}, \frac{1}{4}, \frac{1}{4}$	$\frac{3}{4}, \frac{3}{4}, \frac{1}{4}$	$\frac{1}{4}, \frac{3}{4}, \frac{3}{4}$	$\frac{3}{4}, \frac{1}{4}, \frac{3}{4}$	$hkl: h+k, h+l, k+l=2n$
4	b $\bar{4}$..	$0, 0, 0$	$\frac{1}{2}, \frac{1}{2}, \frac{1}{2}$	$\frac{1}{2}, \frac{1}{2}, 0$	$0, 0, \frac{1}{2}$	$hkl: h+k, l=2n$
4	a 2.. 22	$0, 0, \frac{1}{4}$	$\frac{1}{2}, \frac{1}{2}, \frac{3}{4}$	$\frac{1}{2}, \frac{1}{2}, \frac{1}{4}$	$0, 0, \frac{3}{4}$	$hkl: h+k, l=2n$

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 $0, 0, z$ Along [100] $p2mg$

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

Origin at $x, \frac{1}{4}, 0$ Along [110] $p2mm$

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

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

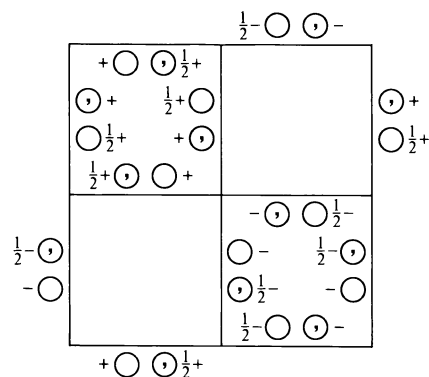
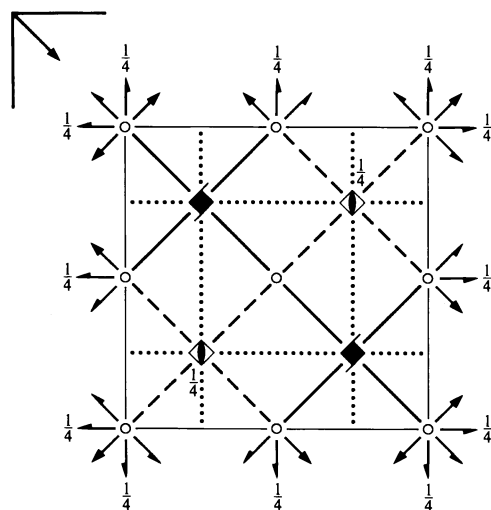
$P4_2/n\bar{c}m$ D_{4h}^{16} $4/m\bar{m}m$

Tetragonal

No. 138

 $P 4_2/n 2_1/c 2/m$ Patterson symmetry $P4/m\bar{m}m$

ORIGIN CHOICE 2

**Origin** at centre $(2/m)$ at $n 1 (2/m, 2_1/g)$, at $\frac{1}{4}, -\frac{1}{4}, \frac{1}{4}$ from $\bar{4}$ **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) $2(0, \frac{1}{2}, 0) 0, y, \frac{1}{4}$ | (6) $2(\frac{1}{2}, 0, 0) x, 0, \frac{1}{4}$ | (7) $2(\frac{1}{2}, \frac{1}{2}, 0) x, x, 0$ | (8) $2 x, \bar{x}, 0$ |
| (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) $c x, \frac{1}{4}, z$ | (14) $c \frac{1}{4}, y, z$ | (15) $m x + \frac{1}{2}, \bar{x}, z$ | (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	<i>j</i> 1	(1) x, y, z (5) $\bar{x}, y + \frac{1}{2}, \bar{z} + \frac{1}{2}$ (9) $\bar{x}, \bar{y}, \bar{z}$ (13) $x, \bar{y} + \frac{1}{2}, z + \frac{1}{2}$	(2) $\bar{x} + \frac{1}{2}, \bar{y} + \frac{1}{2}, z$ (6) $x + \frac{1}{2}, \bar{y}, \bar{z} + \frac{1}{2}$ (10) $x + \frac{1}{2}, y + \frac{1}{2}, \bar{z}$ (14) $\bar{x} + \frac{1}{2}, y, z + \frac{1}{2}$	(3) $\bar{y} + \frac{1}{2}, x, z + \frac{1}{2}$ (7) $y + \frac{1}{2}, x + \frac{1}{2}, \bar{z}$ (11) $y + \frac{1}{2}, \bar{x}, \bar{z} + \frac{1}{2}$ (15) $\bar{y} + \frac{1}{2}, \bar{x} + \frac{1}{2}, z$	(4) $y, \bar{x} + \frac{1}{2}, z + \frac{1}{2}$ (8) $\bar{y}, \bar{x}, \bar{z}$ (12) $\bar{y}, x + \frac{1}{2}, \bar{z} + \frac{1}{2}$ (16) y, x, z	$hk0: h + k = 2n$ $0kl: l = 2n$ $00l: l = 2n$ $h00: h = 2n$
Special: as above, plus						
8	<i>i</i> .. <i>m</i>	x, x, z $\bar{x}, x + \frac{1}{2}, \bar{z} + \frac{1}{2}$	$\bar{x} + \frac{1}{2}, \bar{x} + \frac{1}{2}, z$ $x + \frac{1}{2}, \bar{x}, \bar{z} + \frac{1}{2}$	$\bar{x} + \frac{1}{2}, x, z + \frac{1}{2}$ $x + \frac{1}{2}, x + \frac{1}{2}, \bar{z}$	$x, \bar{x} + \frac{1}{2}, z + \frac{1}{2}$ $\bar{x}, \bar{x}, \bar{z}$	no extra conditions
8	<i>h</i> .. 2	$x, \bar{x}, 0$ $\bar{x}, x, 0$	$\bar{x} + \frac{1}{2}, x + \frac{1}{2}, 0$ $x + \frac{1}{2}, \bar{x} + \frac{1}{2}, 0$	$x + \frac{1}{2}, x, \frac{1}{2}$ $\bar{x} + \frac{1}{2}, \bar{x}, \frac{1}{2}$	$\bar{x}, \bar{x} + \frac{1}{2}, \frac{1}{2}$ $x, x + \frac{1}{2}, \frac{1}{2}$	$hkl: h + k = 2n$
8	<i>g</i> .. 2	$x, \bar{x}, \frac{1}{2}$ $\bar{x}, x, \frac{1}{2}$	$\bar{x} + \frac{1}{2}, x + \frac{1}{2}, \frac{1}{2}$ $x + \frac{1}{2}, \bar{x} + \frac{1}{2}, \frac{1}{2}$	$x + \frac{1}{2}, x, 0$ $\bar{x} + \frac{1}{2}, \bar{x}, 0$	$\bar{x}, \bar{x} + \frac{1}{2}, 0$ $x, x + \frac{1}{2}, 0$	$hkl: h + k = 2n$
8	<i>f</i> 2..	$\frac{3}{4}, \frac{1}{4}, z$ $\frac{1}{4}, \frac{3}{4}, \bar{z}$	$\frac{1}{4}, \frac{3}{4}, z + \frac{1}{2}$ $\frac{3}{4}, \frac{1}{4}, \bar{z} + \frac{1}{2}$	$\frac{1}{4}, \frac{3}{4}, \bar{z} + \frac{1}{2}$ $\frac{3}{4}, \frac{1}{4}, z + \frac{1}{2}$	$\frac{3}{4}, \frac{1}{4}, \bar{z}$ $\frac{1}{4}, \frac{3}{4}, z$	$hkl: h + k, l = 2n$
4	<i>e</i> 2.. <i>mm</i>	$\frac{1}{4}, \frac{1}{4}, z$	$\frac{1}{4}, \frac{1}{4}, z + \frac{1}{2}$	$\frac{3}{4}, \frac{3}{4}, \bar{z} + \frac{1}{2}$	$\frac{3}{4}, \frac{3}{4}, \bar{z}$	$hkl: l = 2n$
4	<i>d</i> .. 2/ <i>m</i>	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	<i>c</i> .. 2/ <i>m</i>	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	<i>b</i> $\bar{4}$..	$\frac{3}{4}, \frac{1}{4}, \frac{3}{4}$	$\frac{1}{4}, \frac{3}{4}, \frac{1}{4}$	$\frac{1}{4}, \frac{3}{4}, \frac{3}{4}$	$\frac{3}{4}, \frac{1}{4}, \frac{1}{4}$	$hkl: h + k, l = 2n$
4	<i>a</i> 2.. 22	$\frac{3}{4}, \frac{1}{4}, 0$	$\frac{1}{4}, \frac{3}{4}, \frac{1}{2}$	$\frac{1}{4}, \frac{3}{4}, 0$	$\frac{3}{4}, \frac{1}{4}, \frac{1}{2}$	$hkl: h + k, l = 2n$

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 $\frac{1}{4}, \frac{1}{4}, z$ Along [100] $p2mg$

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

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

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

Origin at $x, x, 0$