

$P4/nmm$

D_{4h}^7

$4/mmm$

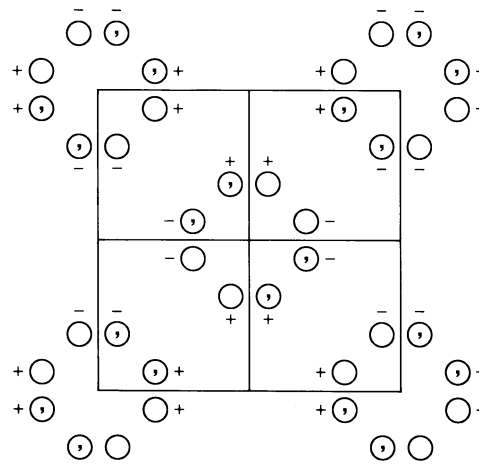
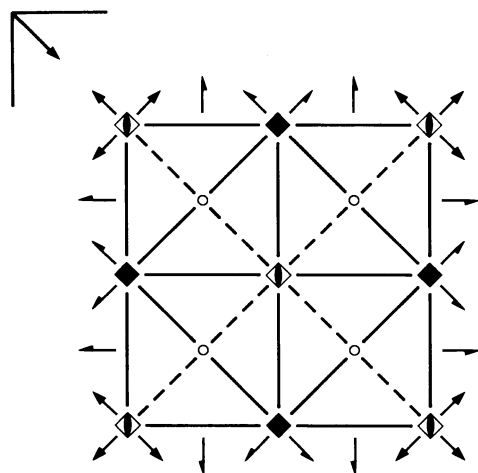
Tetragonal

No. 129

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

Patterson symmetry $P4/mmm$

ORIGIN CHOICE 1



Origin at $\bar{4}m2$ at $\bar{4}/nm2/g$, 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, $\frac{1}{2}$, z | (4) 4 ⁻ $\frac{1}{2}$, 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, 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) 4 ⁺ 0, 0, z; 0, 0, 0 | (12) 4 ⁻ 0, 0, z; 0, 0, 0 |
| (13) m x, 0, z | (14) m 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 <i>k</i> 1	(1) x, y, z (5) $\bar{x} + \frac{1}{2}, y + \frac{1}{2}, \bar{z}$ (9) $\bar{x} + \frac{1}{2}, \bar{y} + \frac{1}{2}, \bar{z}$ (13) x, \bar{y}, z	(2) \bar{x}, \bar{y}, z (6) $x + \frac{1}{2}, \bar{y} + \frac{1}{2}, \bar{z}$ (10) $x + \frac{1}{2}, y + \frac{1}{2}, \bar{z}$ (14) \bar{x}, y, z	(3) $\bar{y} + \frac{1}{2}, x + \frac{1}{2}, z$ (7) y, x, \bar{z} (11) y, \bar{x}, \bar{z} (15) $\bar{y} + \frac{1}{2}, \bar{x} + \frac{1}{2}, z$	(4) $y + \frac{1}{2}, \bar{x} + \frac{1}{2}, z$ (8) $\bar{y}, \bar{x}, \bar{z}$ (12) \bar{y}, x, \bar{z} (16) $y + \frac{1}{2}, x + \frac{1}{2}, z$	$hk0: h + k = 2n$ $h00: h = 2n$
8 <i>j</i> .. <i>m</i>	$x, x + \frac{1}{2}, z$ $\bar{x} + \frac{1}{2}, x, \bar{z}$	$\bar{x}, \bar{x} + \frac{1}{2}, z$ $x + \frac{1}{2}, \bar{x}, \bar{z}$	$\bar{x}, x + \frac{1}{2}, z$ $x + \frac{1}{2}, x, \bar{z}$	$x, \bar{x} + \frac{1}{2}, z$ $\bar{x} + \frac{1}{2}, \bar{x}, \bar{z}$	Special: as above, plus no extra conditions
8 <i>i</i> .. <i>m</i> .	$0, y, z$ $\frac{1}{2}, y + \frac{1}{2}, \bar{z}$	$0, \bar{y}, z$ $\frac{1}{2}, \bar{y} + \frac{1}{2}, \bar{z}$	$\bar{y} + \frac{1}{2}, \frac{1}{2}, z$ $y, 0, \bar{z}$	$y + \frac{1}{2}, \frac{1}{2}, z$ $\bar{y}, 0, \bar{z}$	no extra conditions
8 <i>h</i> .. 2	$x, x, \frac{1}{2}$ $\bar{x} + \frac{1}{2}, \bar{x} + \frac{1}{2}, \frac{1}{2}$	$\bar{x}, \bar{x}, \frac{1}{2}$ $x + \frac{1}{2}, x + \frac{1}{2}, \frac{1}{2}$	$\bar{x} + \frac{1}{2}, x + \frac{1}{2}, \frac{1}{2}$ $x, \bar{x}, \frac{1}{2}$	$x + \frac{1}{2}, \bar{x} + \frac{1}{2}, \frac{1}{2}$ $\bar{x}, x, \frac{1}{2}$	$hkl: h + k = 2n$
8 <i>g</i> .. 2	$x, x, 0$ $\bar{x} + \frac{1}{2}, \bar{x} + \frac{1}{2}, 0$	$\bar{x}, \bar{x}, 0$ $x + \frac{1}{2}, x + \frac{1}{2}, 0$	$\bar{x} + \frac{1}{2}, x + \frac{1}{2}, 0$ $x, \bar{x}, 0$	$x + \frac{1}{2}, \bar{x} + \frac{1}{2}, 0$ $\bar{x}, x, 0$	$hkl: h + k = 2n$
4 <i>f</i> 2 <i>m m</i> .	$0, 0, z$	$\frac{1}{2}, \frac{1}{2}, z$	$\frac{1}{2}, \frac{1}{2}, \bar{z}$	$0, 0, \bar{z}$	$hkl: h + k = 2n$
4 <i>e</i> .. 2/ <i>m</i>	$\frac{1}{4}, \frac{1}{4}, \frac{1}{2}$	$\frac{3}{4}, \frac{3}{4}, \frac{1}{2}$	$\frac{1}{4}, \frac{3}{4}, \frac{1}{2}$	$\frac{3}{4}, \frac{1}{4}, \frac{1}{2}$	$hkl: h, k = 2n$
4 <i>d</i> .. 2/ <i>m</i>	$\frac{1}{4}, \frac{1}{4}, 0$	$\frac{3}{4}, \frac{3}{4}, 0$	$\frac{1}{4}, \frac{3}{4}, 0$	$\frac{3}{4}, \frac{1}{4}, 0$	$hkl: h, k = 2n$
2 <i>c</i> 4 <i>m m</i>	$0, \frac{1}{2}, z$	$\frac{1}{2}, 0, \bar{z}$			no extra conditions
2 <i>b</i> $\bar{4} m 2$	$0, 0, \frac{1}{2}$	$\frac{1}{2}, \frac{1}{2}, \frac{1}{2}$			$hkl: h + k = 2n$
2 <i>a</i> $\bar{4} m 2$	$0, 0, 0$	$\frac{1}{2}, \frac{1}{2}, 0$			$hkl: h + k = 2n$

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] $p2mg$

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

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 $x, x, 0$

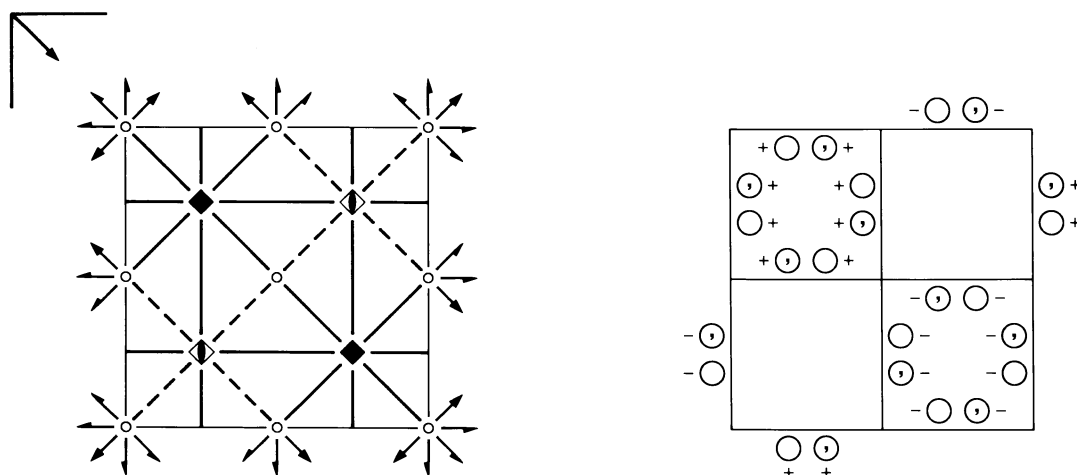
$P4/nmm$ D_{4h}^7 $4/mmm$

Tetragonal

No. 129

 $P 4/n 2_1/m 2/m$ Patterson symmetry $P4/mmm$

ORIGIN CHOICE 2



Origin at centre ($2/m$) at $n2_1(2/m, 2_1/g)$, at $\frac{1}{4}, -\frac{1}{4}, 0$ from $\bar{4}m2$

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) $2(0, \frac{1}{2}, 0) 0, y, 0$ | (6) $2(\frac{1}{2}, 0, 0) x, 0, 0$ | (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) $\bar{4}^+ \frac{1}{4}, -\frac{1}{4}, z; \frac{1}{4}, -\frac{1}{4}, 0$ | (12) $\bar{4}^- -\frac{1}{4}, \frac{1}{4}, z; -\frac{1}{4}, \frac{1}{4}, 0$ |
| (13) $m x, \frac{1}{4}, z$ | (14) $m \frac{1}{4}, y, z$ | (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	k 1	(1) x, y, z (5) $\bar{x}, y + \frac{1}{2}, \bar{z}$ (9) $\bar{x}, \bar{y}, \bar{z}$ (13) $x, \bar{y} + \frac{1}{2}, z$	(2) $\bar{x} + \frac{1}{2}, \bar{y} + \frac{1}{2}, z$ (6) $x + \frac{1}{2}, \bar{y}, \bar{z}$ (10) $x + \frac{1}{2}, y + \frac{1}{2}, \bar{z}$ (14) $\bar{x} + \frac{1}{2}, y, z$	(3) $\bar{y} + \frac{1}{2}, x, z$ (7) $y + \frac{1}{2}, x + \frac{1}{2}, \bar{z}$ (11) $y + \frac{1}{2}, \bar{x}, \bar{z}$ (15) $\bar{y} + \frac{1}{2}, \bar{x} + \frac{1}{2}, z$	(4) $y, \bar{x} + \frac{1}{2}, z$ (8) $\bar{y}, \bar{x}, \bar{z}$ (12) $\bar{y}, x + \frac{1}{2}, \bar{z}$ (16) y, x, z	$hk0: h + k = 2n$ $h00: h = 2n$
8	j $\dots m$	x, x, z $\bar{x}, x + \frac{1}{2}, \bar{z}$	$\bar{x} + \frac{1}{2}, \bar{x} + \frac{1}{2}, z$ $x + \frac{1}{2}, \bar{x}, \bar{z}$	$\bar{x} + \frac{1}{2}, x, z$ $x + \frac{1}{2}, x + \frac{1}{2}, \bar{z}$	$x, \bar{x} + \frac{1}{2}, z$ $\bar{x}, \bar{x}, \bar{z}$	Special: as above, plus no extra conditions
8	i $\dots m$	$\frac{1}{4}, y, z$ $\frac{3}{4}, y + \frac{1}{2}, \bar{z}$	$\frac{1}{4}, \bar{y} + \frac{1}{2}, z$ $\frac{3}{4}, \bar{y}, \bar{z}$	$\bar{y} + \frac{1}{2}, \frac{1}{4}, z$ $y + \frac{1}{2}, \frac{3}{4}, \bar{z}$	$y, \frac{1}{4}, z$ $\bar{y}, \frac{3}{4}, \bar{z}$	no extra conditions
8	h $\dots 2$	$x, \bar{x}, \frac{1}{2}$ $\bar{x}, x, \frac{1}{2}$	$\bar{x} + \frac{1}{2}, x + \frac{1}{2}, \frac{1}{2}$ $x + \frac{1}{2}, \bar{x} + \frac{1}{2}, \frac{1}{2}$	$x + \frac{1}{2}, x, \frac{1}{2}$ $\bar{x} + \frac{1}{2}, \bar{x}, \frac{1}{2}$	$\bar{x}, \bar{x} + \frac{1}{2}, \frac{1}{2}$ $x, x + \frac{1}{2}, \frac{1}{2}$	$hkl: h + k = 2n$
8	g $\dots 2$	$x, \bar{x}, 0$ $\bar{x}, x, 0$	$\bar{x} + \frac{1}{2}, x + \frac{1}{2}, 0$ $x + \frac{1}{2}, \bar{x} + \frac{1}{2}, 0$	$x + \frac{1}{2}, x, 0$ $\bar{x} + \frac{1}{2}, \bar{x}, 0$	$\bar{x}, \bar{x} + \frac{1}{2}, 0$ $x, x + \frac{1}{2}, 0$	$hkl: h + k = 2n$
4	f $2mm$	$\frac{3}{4}, \frac{1}{4}, z$	$\frac{1}{4}, \frac{3}{4}, z$	$\frac{1}{4}, \frac{3}{4}, \bar{z}$	$\frac{3}{4}, \frac{1}{4}, \bar{z}$	$hkl: h + k = 2n$
4	e $\dots 2/m$	$0, 0, \frac{1}{2}$	$\frac{1}{2}, \frac{1}{2}, \frac{1}{2}$	$\frac{1}{2}, 0, \frac{1}{2}$	$0, \frac{1}{2}, \frac{1}{2}$	$hkl: h, k = 2n$
4	d $\dots 2/m$	$0, 0, 0$	$\frac{1}{2}, \frac{1}{2}, 0$	$\frac{1}{2}, 0, 0$	$0, \frac{1}{2}, 0$	$hkl: h, k = 2n$
2	c $4mm$	$\frac{1}{4}, \frac{1}{4}, z$	$\frac{3}{4}, \frac{3}{4}, \bar{z}$			no extra conditions
2	b $\bar{4}m2$	$\frac{3}{4}, \frac{1}{4}, \frac{1}{2}$	$\frac{1}{4}, \frac{3}{4}, \frac{1}{2}$			$hkl: h + k = 2n$
2	a $\bar{4}m2$	$\frac{3}{4}, \frac{1}{4}, 0$	$\frac{1}{4}, \frac{3}{4}, 0$			$hkl: h + k = 2n$

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

Along $[100]$ $p2mg$

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

Origin at $x, 0, 0$

Along $[110]$ $p2mm$

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

Origin at $x, x, 0$