

$P4/ncc$

D_{4h}^8

$4/mmm$

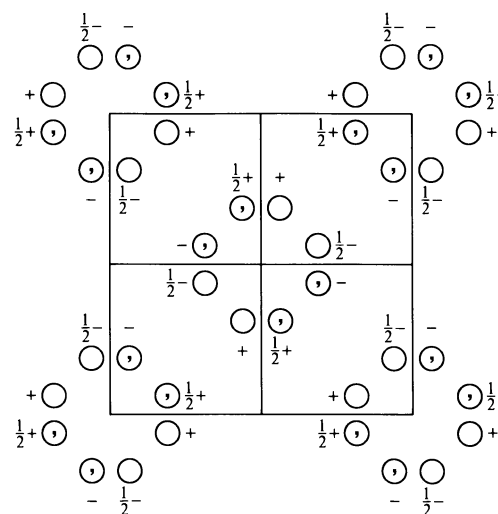
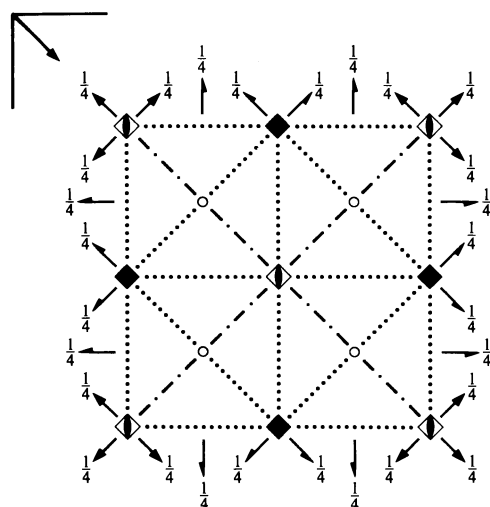
Tetragonal

No. 130

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

Patterson symmetry $P4/mmm$

ORIGIN CHOICE 1



Origin at $\bar{4}/ncn$, at $-\frac{1}{4}, \frac{1}{4}, 0$ 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) $4^+ \ 0, \frac{1}{2}, z$
- (4) $4^- \ \frac{1}{2}, 0, z$
- (5) $2(0, \frac{1}{2}, 0) \ \frac{1}{4}, y, \frac{1}{4}$
- (6) $2(\frac{1}{2}, 0, 0) \ x, \frac{1}{4}, \frac{1}{4}$
- (7) $2 \ x, x, \frac{1}{4}$
- (8) $2 \ x, \bar{x}, \frac{1}{4}$
- (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) $c \ x, 0, z$
- (14) $c \ 0, y, z$
- (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>g</i> 1	(1) x, y, z (2) \bar{x}, \bar{y}, z (3) $\bar{y} + \frac{1}{2}, x + \frac{1}{2}, z$ (4) $y + \frac{1}{2}, \bar{x} + \frac{1}{2}, z$ (5) $\bar{x} + \frac{1}{2}, y + \frac{1}{2}, \bar{z} + \frac{1}{2}$ (6) $x + \frac{1}{2}, \bar{y} + \frac{1}{2}, \bar{z} + \frac{1}{2}$ (7) $y, x, \bar{z} + \frac{1}{2}$ (8) $\bar{y}, \bar{x}, \bar{z} + \frac{1}{2}$ (9) $\bar{x} + \frac{1}{2}, \bar{y} + \frac{1}{2}, \bar{z}$ (10) $x + \frac{1}{2}, y + \frac{1}{2}, \bar{z}$ (11) y, \bar{x}, \bar{z} (12) \bar{y}, x, \bar{z} (13) $x, \bar{y}, z + \frac{1}{2}$ (14) $\bar{x}, y, z + \frac{1}{2}$ (15) $\bar{y} + \frac{1}{2}, \bar{x} + \frac{1}{2}, z + \frac{1}{2}$ (16) $y + \frac{1}{2}, x + \frac{1}{2}, z + \frac{1}{2}$	General: $hk0: h + k = 2n$ $0kl: l = 2n$ $hhl: l = 2n$ $00l: l = 2n$ $h00: h = 2n$
8 <i>f</i> ..2	$x, x, \frac{1}{4}$ $\bar{x}, \bar{x}, \frac{1}{4}$ $x + \frac{1}{2}, \bar{x} + \frac{1}{2}, \frac{3}{4}$ $x + \frac{1}{2}, x + \frac{1}{2}, \frac{3}{4}$	Special: as above, plus $hkl: h + k + l = 2n$
8 <i>e</i> 2..	$0, 0, z$ $\frac{1}{2}, \frac{1}{2}, z$ $\frac{1}{2}, \frac{1}{2}, \bar{z}$ $0, 0, \bar{z}$ $\frac{1}{2}, \frac{1}{2}, \bar{z} + \frac{1}{2}$ $0, 0, z + \frac{1}{2}$ $\frac{1}{2}, \frac{1}{2}, z + \frac{1}{2}$	$hkl: h + k, l = 2n$
8 <i>d</i> $\bar{1}$	$\frac{1}{4}, \frac{1}{4}, 0$ $\frac{3}{4}, \frac{3}{4}, 0$ $\frac{1}{4}, \frac{3}{4}, 0$ $\frac{3}{4}, \frac{1}{4}, 0$ $\frac{1}{4}, \frac{3}{4}, \frac{1}{2}$ $\frac{3}{4}, \frac{1}{4}, \frac{1}{2}$ $\frac{1}{4}, \frac{1}{4}, \frac{1}{2}$ $\frac{3}{4}, \frac{3}{4}, \frac{1}{2}$	$hkl: h, k, l = 2n$
4 <i>c</i> 4..	$0, \frac{1}{2}, z$ $\frac{1}{2}, 0, \bar{z} + \frac{1}{2}$ $\frac{1}{2}, 0, \bar{z}$ $0, \frac{1}{2}, z + \frac{1}{2}$	$hkl: l = 2n$
4 <i>b</i> $\bar{4}$..	$0, 0, 0$ $\frac{1}{2}, \frac{1}{2}, 0$ $\frac{1}{2}, \frac{1}{2}, \frac{1}{2}$ $0, 0, \frac{1}{2}$	$hkl: h + k, l = 2n$
4 <i>a</i> 2.22	$0, 0, \frac{1}{4}$ $\frac{1}{2}, \frac{1}{2}, \frac{1}{4}$ $\frac{1}{2}, \frac{1}{2}, \frac{3}{4}$ $0, 0, \frac{3}{4}$	$hkl: h + k, l = 2n$

Symmetry of special projections

Along $[001] \ p4mm$
 $\mathbf{a}' = \frac{1}{2}(\mathbf{a} - \mathbf{b})$ $\mathbf{b}' = \frac{1}{2}(\mathbf{a} + \mathbf{b})$
 Origin at $0, 0, z$

Along $[100] \ p2mg$
 $\mathbf{a}' = \mathbf{b}$ $\mathbf{b}' = \frac{1}{2}\mathbf{c}$
 Origin at $x, \frac{1}{4}, 0$

Along $[110] \ p2mm$
 $\mathbf{a}' = \frac{1}{2}(-\mathbf{a} + \mathbf{b})$ $\mathbf{b}' = \frac{1}{2}\mathbf{c}$
 Origin at $x, x, 0$

Tetragonal

$4/mmm$

D_{4h}^8

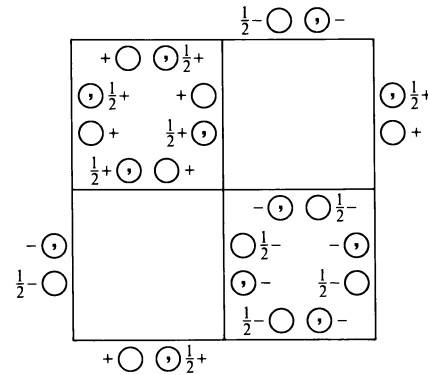
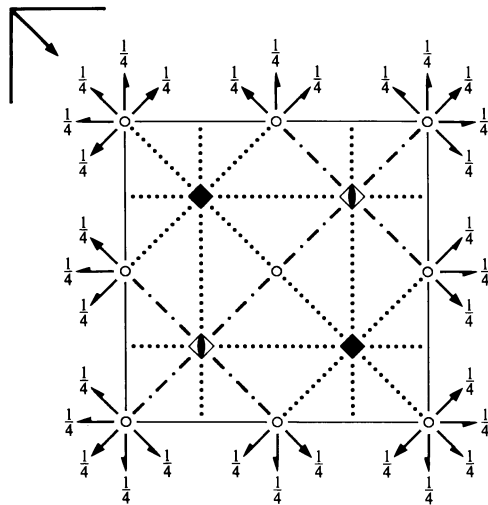
$P4/ncc$

Patterson symmetry $P4/mmm$

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

No. 130

ORIGIN CHOICE 2



Origin at $\bar{1}$ at $n1(c,n)$, at $\frac{1}{4}, -\frac{1}{4}, 0$ from $\bar{4}$

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

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) $2(0, \frac{1}{2}, 0) 0, y, \frac{1}{4}$ | (6) $2(\frac{1}{2}, 0, 0) x, 0, \frac{1}{4}$ | (7) $2(\frac{1}{2}, \frac{1}{2}, 0) x, x, \frac{1}{4}$ | (8) $2 x, \bar{x}, \frac{1}{4}$ |
| (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) $c x, \frac{1}{4}, z$ | (14) $c \frac{1}{4}, y, z$ | (15) $c x + \frac{1}{2}, \bar{x}, z$ | (16) $c x, x, z$ |

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>g</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) $\bar{x}, y + \frac{1}{2}, \bar{z} + \frac{1}{2}$ (6) $x + \frac{1}{2}, \bar{y}, \bar{z} + \frac{1}{2}$ (7) $y + \frac{1}{2}, x + \frac{1}{2}, \bar{z} + \frac{1}{2}$ (8) $\bar{y}, \bar{x}, \bar{z} + \frac{1}{2}$ (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) $x, \bar{y} + \frac{1}{2}, z + \frac{1}{2}$ (14) $\bar{x} + \frac{1}{2}, y, z + \frac{1}{2}$ (15) $\bar{y} + \frac{1}{2}, \bar{x} + \frac{1}{2}, z + \frac{1}{2}$ (16) $y, x, z + \frac{1}{2}$	General: $hkl: h + k = 2n$ $Ok l: l = 2n$ $hhl: l = 2n$ $00l: l = 2n$ $h00: h = 2n$
8 <i>f</i> .. 2	$x, \bar{x}, \frac{1}{4}$ $\bar{x}, x, \frac{3}{4}$ $\bar{x} + \frac{1}{2}, x + \frac{1}{2}, \frac{1}{4}$ $x + \frac{1}{2}, \bar{x} + \frac{1}{2}, \frac{3}{4}$ $x + \frac{1}{2}, x, \frac{1}{4}$ $\bar{x} + \frac{1}{2}, \bar{x}, \frac{3}{4}$ $\bar{x}, \bar{x} + \frac{1}{2}, \frac{1}{4}$ $x, x + \frac{1}{2}, \frac{3}{4}$	Special: as above, plus $hkl: h + k + l = 2n$
8 <i>e</i> 2..	$\frac{3}{4}, \frac{1}{4}, z$ $\frac{1}{4}, \frac{3}{4}, \bar{z}$ $\frac{1}{4}, \frac{3}{4}, z$ $\frac{3}{4}, \frac{1}{4}, \bar{z}$ $\frac{1}{4}, \frac{3}{4}, \bar{z} + \frac{1}{2}$ $\frac{3}{4}, \frac{1}{4}, z + \frac{1}{2}$ $\frac{3}{4}, \frac{1}{4}, z$ $\frac{1}{4}, \frac{3}{4}, \bar{z} + \frac{1}{2}$ $\frac{3}{4}, \frac{1}{4}, z + \frac{1}{2}$	$hkl: h + k, l = 2n$
8 <i>d</i> $\bar{1}$	$0, 0, 0$ $\frac{1}{2}, \frac{1}{2}, 0$ $\frac{1}{2}, 0, 0$ $0, \frac{1}{2}, 0$ $0, \frac{1}{2}, \frac{1}{2}$ $\frac{1}{2}, 0, \frac{1}{2}$ $\frac{1}{2}, \frac{1}{2}, \frac{1}{2}$ $0, 0, \frac{1}{2}$	$hkl: h, k, l = 2n$
4 <i>c</i> 4..	$\frac{1}{4}, \frac{1}{4}, z$ $\frac{3}{4}, \frac{3}{4}, \bar{z} + \frac{1}{2}$ $\frac{3}{4}, \frac{3}{4}, \bar{z}$ $\frac{1}{4}, \frac{1}{4}, z + \frac{1}{2}$	$hkl: l = 2n$
4 <i>b</i> $\bar{4}$..	$\frac{3}{4}, \frac{1}{4}, 0$ $\frac{1}{4}, \frac{3}{4}, 0$ $\frac{1}{4}, \frac{3}{4}, \frac{1}{2}$ $\frac{3}{4}, \frac{1}{4}, \frac{1}{2}$	$hkl: h + k, l = 2n$
4 <i>a</i> 2.22	$\frac{3}{4}, \frac{1}{4}, \frac{1}{4}$ $\frac{1}{4}, \frac{3}{4}, \frac{1}{4}$ $\frac{1}{4}, \frac{3}{4}, \frac{3}{4}$ $\frac{3}{4}, \frac{1}{4}, \frac{3}{4}$	$hkl: h + k, l = 2n$

Symmetry of special projections

Along $[001] p4mm$

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

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

Along $[100] p2mg$

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

Origin at $x, 0, 0$

Along $[110] p2mm$

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

Origin at $x, x, 0$