

$P4/n$

$C_{4h}^3$

$4/m$

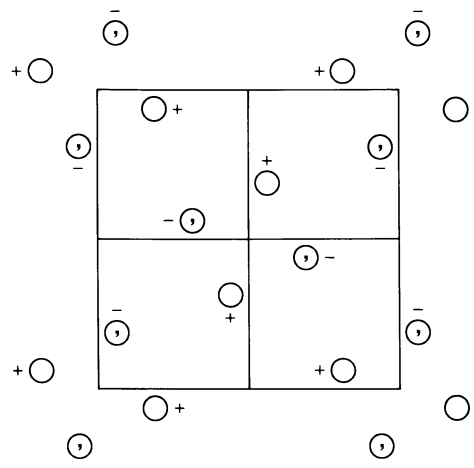
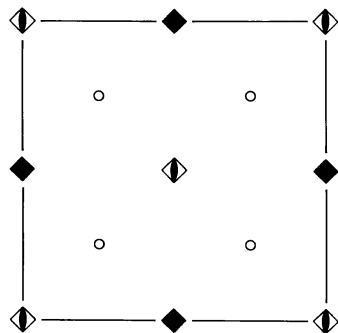
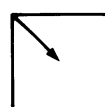
Tetragonal

No. 85

$P4/n$

Patterson symmetry  $P4/m$

ORIGIN CHOICE 1



Origin at  $\bar{4}$  on  $n$ , at  $-\frac{1}{4}, \frac{1}{4}, 0$  from  $\bar{1}$

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

Symmetry operations

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

Generators selected (1);  $t(1, 0, 0)$ ;  $t(0, 1, 0)$ ;  $t(0, 0, 1)$ ; (2); (3); (5)

Positions

Multiplicity, Wyckoff letter, Site symmetry	Coordinates	Reflection conditions
8 <i>g</i> 1	(1) $x, y, z$ (5) $\bar{x} + \frac{1}{2}, \bar{y} + \frac{1}{2}, \bar{z}$ (2) $\bar{x}, \bar{y}, z$ (6) $x + \frac{1}{2}, y + \frac{1}{2}, \bar{z}$ (3) $\bar{y} + \frac{1}{2}, x + \frac{1}{2}, z$ (7) $y, \bar{x}, \bar{z}$ (4) $y + \frac{1}{2}, \bar{x} + \frac{1}{2}, z$ (8) $\bar{y}, x, \bar{z}$	General: $hk0: h + k = 2n$ $h00: h = 2n$
4 <i>f</i> 2..	$0, 0, z$ $\frac{1}{2}, \frac{1}{2}, z$ $\frac{1}{2}, \frac{1}{2}, \bar{z}$ $0, 0, \bar{z}$	Special: as above, plus $hkl: h + k = 2n$
4 <i>e</i> $\bar{1}$	$\frac{1}{4}, \frac{1}{4}, \frac{1}{2}$ $\frac{3}{4}, \frac{3}{4}, \frac{1}{2}$ $\frac{1}{4}, \frac{3}{4}, \frac{1}{2}$ $\frac{3}{4}, \frac{1}{4}, \frac{1}{2}$	$hkl: h, k = 2n$
4 <i>d</i> $\bar{1}$	$\frac{1}{4}, \frac{1}{4}, 0$ $\frac{3}{4}, \frac{3}{4}, 0$ $\frac{1}{4}, \frac{3}{4}, 0$ $\frac{3}{4}, \frac{1}{4}, 0$	$hkl: h, k = 2n$
2 <i>c</i> 4..	$0, \frac{1}{2}, z$ $\frac{1}{2}, 0, \bar{z}$	no extra conditions
2 <i>b</i> $\bar{4}$ ..	$0, 0, \frac{1}{2}$ $\frac{1}{2}, \frac{1}{2}, \frac{1}{2}$	$hkl: h + k = 2n$
2 <i>a</i> $\bar{4}$ ..	$0, 0, 0$ $\frac{1}{2}, \frac{1}{2}, 0$	$hkl: h + k = 2n$

Symmetry of special projections

Along  $[001] \ p4$

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

Origin at  $0, 0, z$

Along  $[100] \ p2mg$

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

Origin at  $x, \frac{1}{4}, 0$

Along  $[110] \ p2mm$

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

Origin at  $x, x, 0$

Tetragonal

$4/m$

$C_{4h}^3$

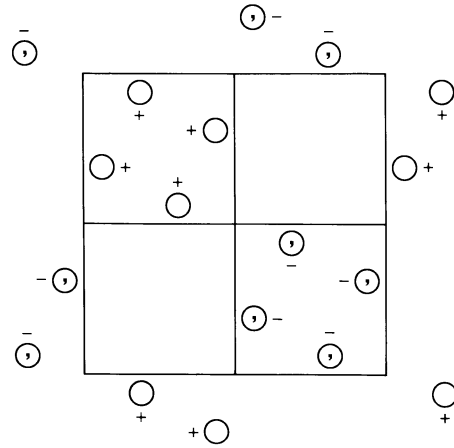
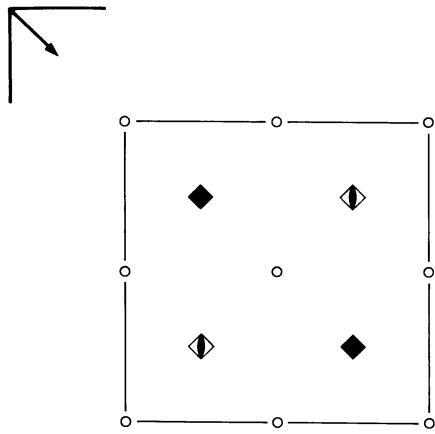
$P4/n$

Patterson symmetry  $P4/m$

$P4/n$

No. 85

ORIGIN CHOICE 2



Origin at  $\bar{1}$  on  $n$ , at  $\frac{1}{4}, -\frac{1}{4}, 0$  from  $\bar{4}$

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

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)  $\bar{1} 0, 0, 0$  (6)  $n(\frac{1}{2}, \frac{1}{2}, 0) x, y, 0$  (7)  $\bar{4}^+ \frac{1}{4}, -\frac{1}{4}, z; \frac{1}{4}, -\frac{1}{4}, 0$  (8)  $\bar{4}^- -\frac{1}{4}, \frac{1}{4}, z; -\frac{1}{4}, \frac{1}{4}, 0$

Generators selected (1);  $t(1, 0, 0)$ ;  $t(0, 1, 0)$ ;  $t(0, 0, 1)$ ; (2); (3); (5)

Positions

Multiplicity, Wyckoff letter, Site symmetry	Coordinates	Reflection conditions
8 $g$ 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) $\bar{x}, \bar{y}, \bar{z}$ (6) $x + \frac{1}{2}, y + \frac{1}{2}, \bar{z}$ (7) $y + \frac{1}{2}, \bar{x}, \bar{z}$ (8) $\bar{y}, x + \frac{1}{2}, \bar{z}$	General: $hk0: h + k = 2n$ $h00: h = 2n$
4 $f$ 2..	$\frac{1}{4}, \frac{3}{4}, z$ $\frac{3}{4}, \frac{1}{4}, z$ $\frac{3}{4}, \frac{1}{4}, \bar{z}$ $\frac{1}{4}, \frac{3}{4}, \bar{z}$	Special: as above, plus $hkl: h + k = 2n$
4 $e$ $\bar{1}$	$0, 0, \frac{1}{2}$ $\frac{1}{2}, \frac{1}{2}, \frac{1}{2}$ $\frac{1}{2}, 0, \frac{1}{2}$ $0, \frac{1}{2}, \frac{1}{2}$	$hkl: h, k = 2n$
4 $d$ $\bar{1}$	$0, 0, 0$ $\frac{1}{2}, \frac{1}{2}, 0$ $\frac{1}{2}, 0, 0$ $0, \frac{1}{2}, 0$	$hkl: h, k = 2n$
2 $c$ 4..	$\frac{1}{4}, \frac{1}{4}, z$ $\frac{3}{4}, \frac{3}{4}, \bar{z}$	no extra conditions
2 $b$ $\bar{4}$ ..	$\frac{1}{4}, \frac{3}{4}, \frac{1}{2}$ $\frac{3}{4}, \frac{1}{4}, \frac{1}{2}$	$hkl: h + k = 2n$
2 $a$ $\bar{4}$ ..	$\frac{1}{4}, \frac{3}{4}, 0$ $\frac{3}{4}, \frac{1}{4}, 0$	$hkl: h + k = 2n$

Symmetry of special projections

Along  $[001]$   $p4$   
 $\mathbf{a}' = \frac{1}{2}(\mathbf{a} - \mathbf{b})$   $\mathbf{b}' = \frac{1}{2}(\mathbf{a} + \mathbf{b})$   
 Origin at  $\frac{1}{4}, \frac{1}{4}, z$

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

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