

$P4_2/n$

$C_{4h}^4$

$4/m$

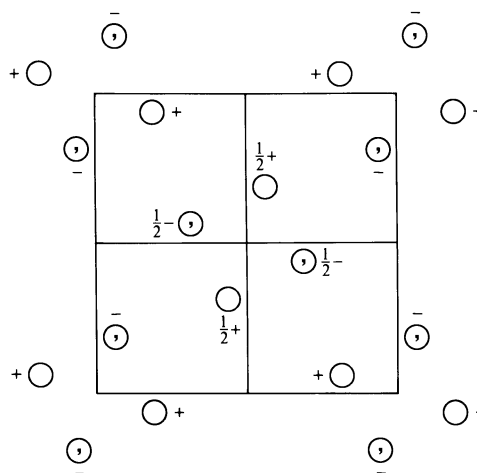
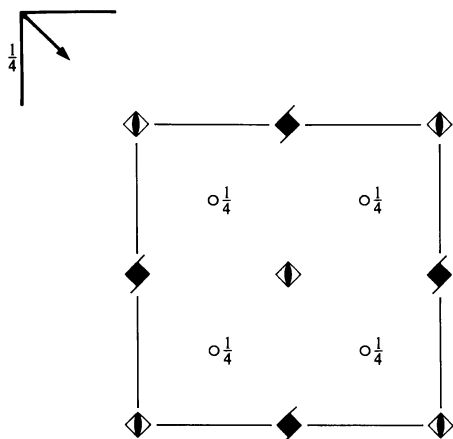
Tetragonal

No. 86

$P4_2/n$

Patterson symmetry  $P4/m$

ORIGIN CHOICE 1



**Origin** at  $\bar{4}$ , at  $-\frac{1}{4}, -\frac{1}{4}, -\frac{1}{4}$  from  $\bar{1}$

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

**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) $\bar{1} \ \frac{1}{4}, \frac{1}{4}, \frac{1}{4}$ | (6) $n(\frac{1}{2}, \frac{1}{2}, 0) \ x, y, \frac{1}{4}$ | (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
					General:
8 <i>g</i> 1	(1) $x, y, z$ (5) $\bar{x} + \frac{1}{2}, \bar{y} + \frac{1}{2}, \bar{z} + \frac{1}{2}$	(2) $\bar{x}, \bar{y}, z$ (6) $x + \frac{1}{2}, y + \frac{1}{2}, \bar{z} + \frac{1}{2}$	(3) $\bar{y} + \frac{1}{2}, x + \frac{1}{2}, z + \frac{1}{2}$ (7) $y, \bar{x}, \bar{z}$	(4) $y + \frac{1}{2}, \bar{x} + \frac{1}{2}, z + \frac{1}{2}$ (8) $\bar{y}, x, \bar{z}$	$hk0 : h + k = 2n$ $00l : l = 2n$ $h00 : h = 2n$
					Special: as above, plus
4 <i>f</i> 2..	0, 0, $z$	$\frac{1}{2}, \frac{1}{2}, z + \frac{1}{2}$	$\frac{1}{2}, \frac{1}{2}, \bar{z} + \frac{1}{2}$	0, 0, $\bar{z}$	$hkl : h + k + l = 2n$
4 <i>e</i> 2..	0, $\frac{1}{2}, z$	0, $\frac{1}{2}, z + \frac{1}{2}$	$\frac{1}{2}, 0, \bar{z} + \frac{1}{2}$	$\frac{1}{2}, 0, \bar{z}$	$hkl : l = 2n$
4 <i>d</i> $\bar{1}$	$\frac{1}{4}, \frac{1}{4}, \frac{3}{4}$	$\frac{3}{4}, \frac{3}{4}, \frac{3}{4}$	$\frac{1}{4}, \frac{3}{4}, \frac{1}{4}$	$\frac{3}{4}, \frac{1}{4}, \frac{1}{4}$	$hkl : h + k, h + l, k + l = 2n$
4 <i>c</i> $\bar{1}$	$\frac{1}{4}, \frac{1}{4}, \frac{1}{4}$	$\frac{3}{4}, \frac{3}{4}, \frac{1}{4}$	$\frac{1}{4}, \frac{3}{4}, \frac{3}{4}$	$\frac{3}{4}, \frac{1}{4}, \frac{3}{4}$	$hkl : h + k, h + l, k + l = 2n$
2 <i>b</i> $\bar{4}$ ..	0, 0, $\frac{1}{2}$	$\frac{1}{2}, \frac{1}{2}, 0$			$hkl : h + k + l = 2n$
2 <i>a</i> $\bar{4}$ ..	0, 0, 0	$\frac{1}{2}, \frac{1}{2}, \frac{1}{2}$			$hkl : h + k + l = 2n$

**Symmetry of special projections**

Along [001]  $p4$

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

Origin at 0, 0,  $z$

Along [100]  $p2mg$

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

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

Along [110]  $p2mm$

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

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

**Maximal non-isomorphic subgroups**

- I** [2]  $P\bar{4}$  (81) 1; 2; 7; 8  
 [2]  $P4_2$  (77) 1; 2; 3; 4  
 [2]  $P2/n$  ( $P2/c$ , 13) 1; 2; 5; 6

**IIa** none

**IIb** [2]  $F4_1/d$  ( $\mathbf{a}' = 2\mathbf{a}, \mathbf{b}' = 2\mathbf{b}, \mathbf{c}' = 2\mathbf{c}$ ) ( $I4_1/a$ , 88)

**Maximal isomorphic subgroups of lowest index**

**IIc** [3]  $P4_2/n$  ( $\mathbf{c}' = 3\mathbf{c}$ ) (86); [5]  $P4_2/n$  ( $\mathbf{a}' = \mathbf{a} + 2\mathbf{b}, \mathbf{b}' = -2\mathbf{a} + \mathbf{b}$  or  $\mathbf{a}' = \mathbf{a} - 2\mathbf{b}, \mathbf{b}' = 2\mathbf{a} + \mathbf{b}$ ) (86)

**Minimal non-isomorphic supergroups**

**I** [2]  $P4_2/nbc$  (133); [2]  $P4_2/nnm$  (134); [2]  $P4_2/nmc$  (137); [2]  $P4_2/ncm$  (138)

**II** [2]  $C4_2/m$  ( $P4_2/m$ , 84); [2]  $I4/m$  (87); [2]  $P4/n$  ( $\mathbf{c}' = \frac{1}{2}\mathbf{c}$ ) (85)

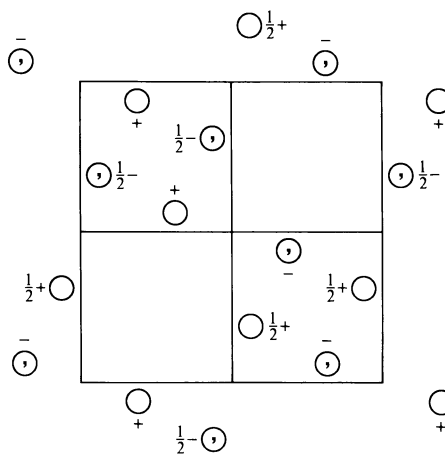
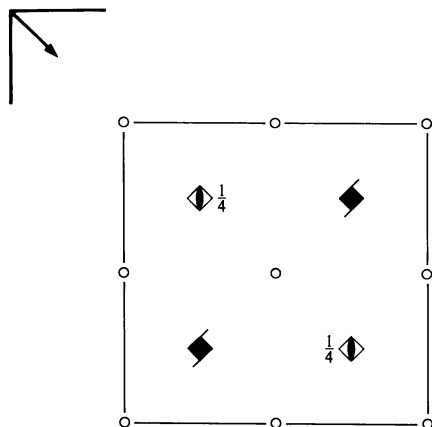
$P4_2/n$  $C_{4h}^4$  $4/m$ 

Tetragonal

No. 86

 $P4_2/n$ Patterson symmetry  $P4/m$ 

ORIGIN CHOICE 2

Origin at  $\bar{1}$  on  $n$ , at  $\frac{1}{4}, \frac{1}{4}, \frac{1}{4}$  from  $\bar{4}$ Asymmetric unit  $-\frac{1}{4} \leq x \leq \frac{1}{4}; -\frac{1}{4} \leq y \leq \frac{1}{4}; 0 \leq z \leq \frac{1}{2}$ 

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

**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) $x, y, z$ (5) $\bar{x}, \bar{y}, \bar{z}$	(2) $\bar{x} + \frac{1}{2}, \bar{y} + \frac{1}{2}, z$ (6) $x + \frac{1}{2}, y + \frac{1}{2}, \bar{z}$	(3) $\bar{y}, x + \frac{1}{2}, z + \frac{1}{2}$ (7) $y, \bar{x} + \frac{1}{2}, \bar{z} + \frac{1}{2}$	(4) $y + \frac{1}{2}, \bar{x}, z + \frac{1}{2}$ (8) $\bar{y} + \frac{1}{2}, x, \bar{z} + \frac{1}{2}$	General: $hk0 : h + k = 2n$ $00l : l = 2n$ $h00 : h = 2n$ Special: as above, plus $hkl : h + k + l = 2n$
4	$f$ 2..	$\frac{1}{4}, \frac{1}{4}, z$	$\frac{3}{4}, \frac{3}{4}, z + \frac{1}{2}$	$\frac{3}{4}, \frac{3}{4}, \bar{z}$	$\frac{1}{4}, \frac{1}{4}, \bar{z} + \frac{1}{2}$	$hkl : h + k + l = 2n$
4	$e$ 2..	$\frac{3}{4}, \frac{1}{4}, z$	$\frac{3}{4}, \frac{1}{4}, z + \frac{1}{2}$	$\frac{1}{4}, \frac{3}{4}, \bar{z}$	$\frac{1}{4}, \frac{3}{4}, \bar{z} + \frac{1}{2}$	$hkl : l = 2n$
4	$d$ $\bar{1}$	$0, 0, \frac{1}{2}$	$\frac{1}{2}, \frac{1}{2}, \frac{1}{2}$	$0, \frac{1}{2}, 0$	$\frac{1}{2}, 0, 0$	$hkl : h + k, h + l, k + l = 2n$
4	$c$ $\bar{1}$	$0, 0, 0$	$\frac{1}{2}, \frac{1}{2}, 0$	$0, \frac{1}{2}, \frac{1}{2}$	$\frac{1}{2}, 0, \frac{1}{2}$	$hkl : h + k, h + l, k + l = 2n$
2	$b$ $\bar{4}$ ..	$\frac{1}{4}, \frac{1}{4}, \frac{3}{4}$	$\frac{3}{4}, \frac{3}{4}, \frac{1}{4}$			$hkl : h + k + l = 2n$
2	$a$ $\bar{4}$ ..	$\frac{1}{4}, \frac{1}{4}, \frac{1}{4}$	$\frac{3}{4}, \frac{3}{4}, \frac{3}{4}$			$hkl : h + k + l = 2n$

**Symmetry of special projections**

Along  $[001]$   $p4$

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

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  $x, x, 0$

**Maximal non-isomorphic subgroups**

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 [2]  $P4_2$  (77) 1; 2; 3; 4  
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