

$p4/n$

$4/m$

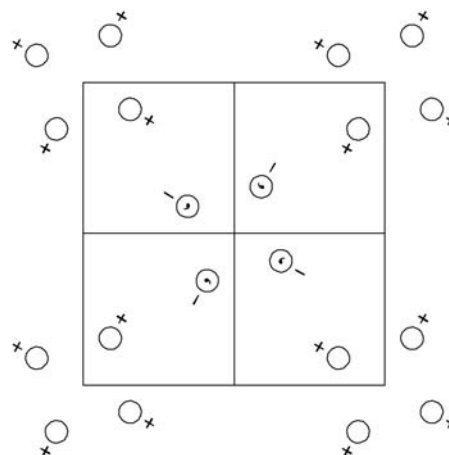
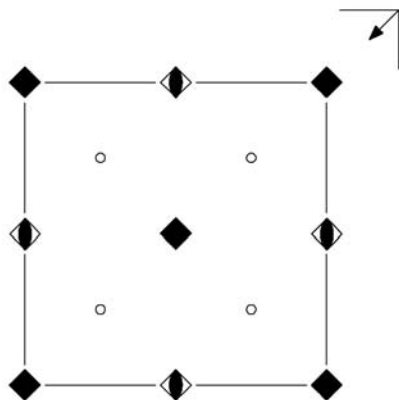
Tetragonal/Square

No. 52

$p4/n$

Patterson symmetry  $p4/m$

ORIGIN CHOICE 1



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

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

Symmetry operations

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

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

**Positions**

Multiplicity, Wyckoff letter, Site symmetry	Coordinates				Reflection conditions
					General:
8 <i>e</i> 1	(1) $x, y, z$	(2) $\bar{x}, \bar{y}, z$	(3) $\bar{y}, x, z$	(4) $y, \bar{x}, z$	$hk: h+k=2n$
	(5) $\bar{x}+\frac{1}{2}, \bar{y}+\frac{1}{2}, \bar{z}$	(6) $x+\frac{1}{2}, y+\frac{1}{2}, \bar{z}$	(7) $y+\frac{1}{2}, \bar{x}+\frac{1}{2}, \bar{z}$	(8) $\bar{y}+\frac{1}{2}, x+\frac{1}{2}, \bar{z}$	$h0: h=2n$ $0k: k=2n$
4 <i>d</i> 2..	$\frac{1}{2}, 0, z$	$0, \frac{1}{2}, z$	$0, \frac{1}{2}, \bar{z}$	$\frac{1}{2}, 0, \bar{z}$	Special: as above, plus no extra conditions
4 <i>c</i> $\bar{1}$	$\frac{1}{4}, \frac{1}{4}, 0$	$\frac{3}{4}, \frac{3}{4}, 0$	$\frac{3}{4}, \frac{1}{4}, 0$	$\frac{1}{4}, \frac{3}{4}, 0$	$hk: h, k=2n$
2 <i>b</i> 4..	$\frac{1}{2}, \frac{1}{2}, z$	$0, 0, \bar{z}$			no extra conditions
2 <i>a</i> $\bar{4}$ ..	$\frac{1}{2}, 0, 0$	$0, \frac{1}{2}, 0$			no extra conditions

**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]  $\neq 2mg$

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

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

Along [110]  $\neq 2mm$

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

Origin at  $x, x, 0$

**Maximal non-isotypic subgroups**

<b>I</b>	[2] $p\bar{4}$ (50)	1; 2; 7; 8
	[2] $p4$ (49)	1; 2; 3; 4
	[2] $p2/n11$ ( $p112/a, 7$ )	1; 2; 5; 6

**IIa** none

**IIb** none

**Maximal isotypic subgroups of lowest index**

**IIc** [5]  $p4/n$  ( $\mathbf{a}' = \mathbf{a} + 2\mathbf{b}, \mathbf{b}' = -2\mathbf{a} + \mathbf{b}$  or  $\mathbf{a}' = \mathbf{a} - 2\mathbf{b}, \mathbf{b}' = 2\mathbf{a} + \mathbf{b}$ ) (52)

**Minimal non-isotypic supergroups**

**I** [2]  $p4/nbm$  (62); [2]  $p4/nmm$  (64)

**II** [2]  $c4/m$  ( $p4/m, 51$ )

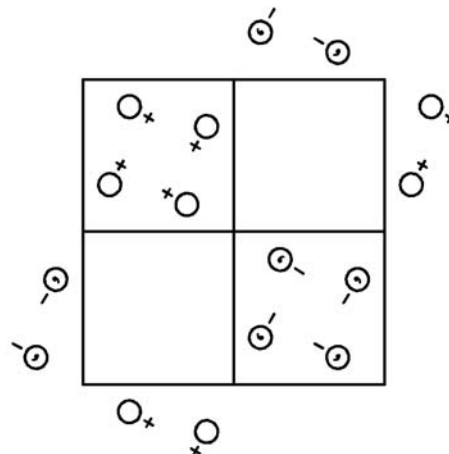
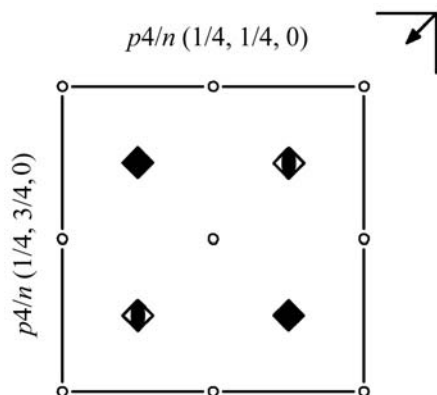
$p4/n (\frac{1}{4}, \frac{1}{4}, 0)$  $4/m$ 

Tetragonal/Square

No. 52

 $p4/n$ Patterson symmetry  $p4/m$ 

ORIGIN CHOICE 2

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

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

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

**Positions**

Multiplicity, Wyckoff letter, Site symmetry	Coordinates				Reflection conditions
8 <i>e</i> 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) $\bar{y} + \frac{1}{2}, x, z$ (7) $y + \frac{1}{2}, \bar{x}, \bar{z}$	(4) $y, \bar{x} + \frac{1}{2}, z$ (8) $\bar{y}, x + \frac{1}{2}, \bar{z}$	General: $hk: h + k = 2n$ $h0: h = 2n$ $0k: k = 2n$ Special: as above, plus
4 <i>d</i> 2..	$\frac{1}{4}, \frac{3}{4}, z$	$\frac{3}{4}, \frac{1}{4}, z$	$\frac{3}{4}, \frac{1}{4}, \bar{z}$	$\frac{1}{4}, \frac{3}{4}, \bar{z}$	no extra conditions
4 <i>c</i> $\bar{1}$	0,0,0	$\frac{1}{2}, \frac{1}{2}, 0$	$\frac{1}{2}, 0, 0$	$0, \frac{1}{2}, 0$	$hk: h, k = 2n$
2 <i>b</i> 4..	$\frac{1}{4}, \frac{1}{4}, z$	$\frac{3}{4}, \frac{3}{4}, \bar{z}$			no extra conditions
2 <i>a</i> $\bar{4}$ ..	$\frac{1}{4}, \frac{3}{4}, 0$	$\frac{3}{4}, \frac{1}{4}, 0$			no extra conditions

**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]  $\neq 2mg$

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

Origin at  $x, 0, 0$

Along [110]  $\neq 2mm$

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

Origin at  $x, x, 0$

**Maximal non-isotypic subgroups**

<b>I</b>	[2] $p\bar{4}$ (50)	1; 2; 7; 8
	[2] $p4$ (49)	1; 2; 3; 4
	[2] $p2/n11$ ( $p112/a, 7$ )	1; 2; 5; 6

**IIa** none

**IIb** none

**Maximal isotypic subgroups of lowest index**

**IIc** [5]  $p4/n$  ( $\mathbf{a}' = \mathbf{a} + 2\mathbf{b}, \mathbf{b}' = -2\mathbf{a} + \mathbf{b}$  or  $\mathbf{a}' = \mathbf{a} - 2\mathbf{b}, \mathbf{b}' = 2\mathbf{a} + \mathbf{b}$ ) (52)

**Minimal non-isotypic supergroups**

**I** [2]  $p4/nbm$  (62); [2]  $p4/nmm$  (64)

**II** [2]  $c4/m$  ( $p4/m, 51$ )