

$p\bar{4}2_1m$

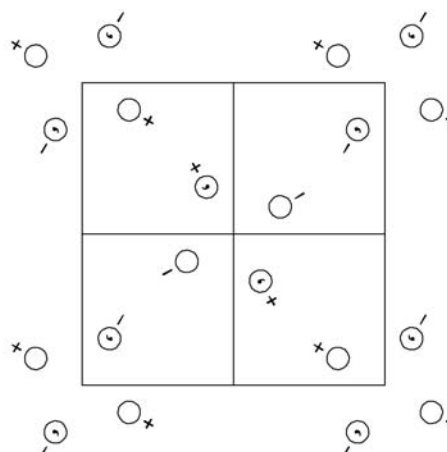
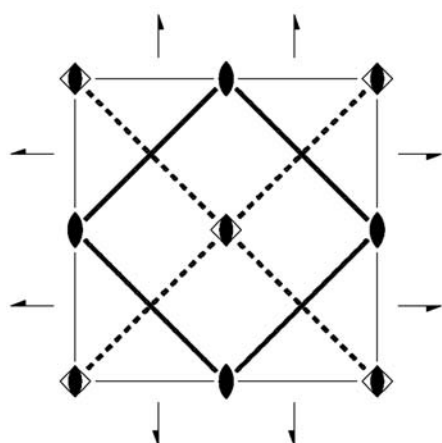
$\bar{4}2m$

Tetragonal/Square

No. 58

$p\bar{4}2_1m$

Patterson symmetry  $p4/mmm$



Origin at  $\bar{4}1g$

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

Symmetry operations

- |  |  |                                     |  |
|--|--|-------------------------------------|--|
| (1) 1  | (2) 2 $0,0,z$                                | (3) $\bar{4}^+ 0,0,z; 0,0,0$        | (4) $\bar{4}^- 0,0,z; 0,0,0$                 |
| (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) $m x + \frac{1}{2}, \bar{x}, z$ | (8) $g(\frac{1}{2}, \frac{1}{2}, 0) x, x, z$ |

**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) $x, y, z$ (5) $\bar{x} + \frac{1}{2}, y + \frac{1}{2}, \bar{z}$	(2) $\bar{x}, \bar{y}, z$ (6) $x + \frac{1}{2}, \bar{y} + \frac{1}{2}, \bar{z}$	(3) $y, \bar{x}, \bar{z}$ (7) $\bar{y} + \frac{1}{2}, \bar{x} + \frac{1}{2}, z$	(4) $\bar{y}, x, \bar{z}$ (8) $y + \frac{1}{2}, x + \frac{1}{2}, z$	$h0: h = 2n$
4 <i>d</i> $\dots m$	$x, x + \frac{1}{2}, z$	$\bar{x}, \bar{x} + \frac{1}{2}, z$	$x + \frac{1}{2}, \bar{x}, \bar{z}$	$\bar{x} + \frac{1}{2}, x, \bar{z}$	Special: as above, plus no extra conditions
4 <i>c</i> $2 \dots$	$0, 0, z$	$0, 0, \bar{z}$	$\frac{1}{2}, \frac{1}{2}, \bar{z}$	$\frac{1}{2}, \frac{1}{2}, z$	$hk: h + k = 2n$
2 <i>b</i> $2 \dots mm$	$0, \frac{1}{2}, z$	$\frac{1}{2}, 0, \bar{z}$			$hk: h + k = 2n$
2 <i>a</i> $\bar{4} \dots$	$0, 0, 0$	$\frac{1}{2}, \frac{1}{2}, 0$			$hk: h + k = 2n$

**Symmetry of special projections**

Along  $[001] p4gm$

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

Origin at  $0, 0, z$

Along  $[100] \not p2mg$

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

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

Along  $[110] \not p1m1$

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

Origin at  $x, x, 0$

**Maximal non-isotypic subgroups**

<b>I</b>	$[2] p\bar{4}11 (p\bar{4}, 50)$	1; 2; 3; 4
	$[2] p21m (cmm2, 26)$	1; 2; 7; 8
	$[2] p22_11 (p2_12_12, 21)$	1; 2; 5; 6

**IIa** none

**IIb** none

**Maximal isotypic subgroups of lowest index**

**IIc**  $[9] p\bar{4}2_1m (\mathbf{a}' = 3\mathbf{a}, \mathbf{b}' = 3\mathbf{b}) (58)$

**Minimal non-isotypic supergroups**

**I**  $[2] p4/mbm (63)$ ;  $[2] p4/nmm (64)$

**II**  $[2] c\bar{4}2m (p\bar{4}m2, 59)$