

$P4_2 2_1 2$

$D_4^6$

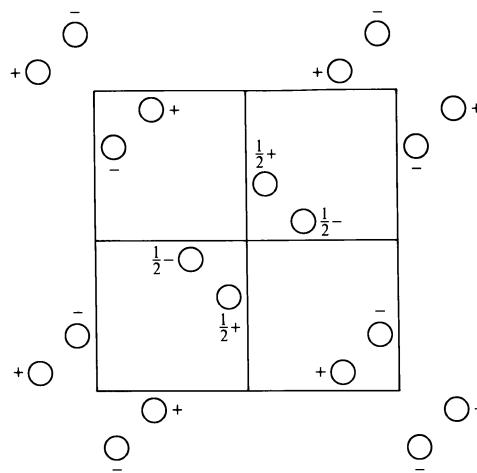
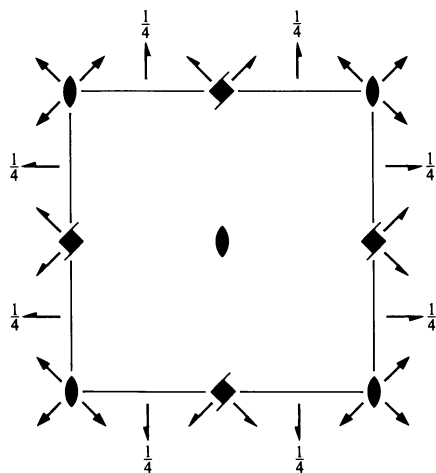
422

Tetragonal

No. 94

$P4_2 2_1 2$

Patterson symmetry  $P4/mmm$



Origin at 222 at 212

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

**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) $\bar{x} + \frac{1}{2}, y + \frac{1}{2}, \bar{z} + \frac{1}{2}$	(2) $\bar{x}, \bar{y}, z$ (6) $x + \frac{1}{2}, \bar{y} + \frac{1}{2}, \bar{z} + \frac{1}{2}$	(3) $\bar{y} + \frac{1}{2}, x + \frac{1}{2}, z + \frac{1}{2}$ (7) $y, x, \bar{z}$	(4) $y + \frac{1}{2}, \bar{x} + \frac{1}{2}, z + \frac{1}{2}$ (8) $\bar{y}, \bar{x}, \bar{z}$	$00l : l = 2n$ $h00 : h = 2n$
					Special: as above, plus
4 <i>f</i> ..2	$x, x, \frac{1}{2}$	$\bar{x}, \bar{x}, \frac{1}{2}$	$\bar{x} + \frac{1}{2}, x + \frac{1}{2}, 0$	$x + \frac{1}{2}, \bar{x} + \frac{1}{2}, 0$	$0kl : k + l = 2n$
4 <i>e</i> ..2	$x, x, 0$	$\bar{x}, \bar{x}, 0$	$\bar{x} + \frac{1}{2}, x + \frac{1}{2}, \frac{1}{2}$	$x + \frac{1}{2}, \bar{x} + \frac{1}{2}, \frac{1}{2}$	$0kl : k + l = 2n$
4 <i>d</i> 2..	$0, \frac{1}{2}, z$	$0, \frac{1}{2}, z + \frac{1}{2}$	$\frac{1}{2}, 0, \bar{z} + \frac{1}{2}$	$\frac{1}{2}, 0, \bar{z}$	$hkl : l = 2n$ $hk0 : h + k = 2n$
4 <i>c</i> 2..	$0, 0, z$	$\frac{1}{2}, \frac{1}{2}, z + \frac{1}{2}$	$\frac{1}{2}, \frac{1}{2}, \bar{z} + \frac{1}{2}$	$0, 0, \bar{z}$	$hkl : h + k + l = 2n$
2 <i>b</i> 2.22	$0, 0, \frac{1}{2}$	$\frac{1}{2}, \frac{1}{2}, 0$			$hkl : h + k + l = 2n$
2 <i>a</i> 2.22	$0, 0, 0$	$\frac{1}{2}, \frac{1}{2}, \frac{1}{2}$			$hkl : h + k + l = 2n$

**Symmetry of special projections**

Along [001]  $p4gm$

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

Origin at  $0, \frac{1}{2}, z$

Along [100]  $p2mg$

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

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

Along [110]  $p2mm$

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

Origin at  $x, x, 0$

**Maximal non-isomorphic subgroups**

- I** [2]  $P4_2 11$  ( $P4_2, 77$ ) 1; 2; 3; 4  
 [2]  $P2 12$  ( $C2 22, 21$ ) 1; 2; 7; 8  
 [2]  $P2 2_1 1$  ( $P2_1 2_1 2, 18$ ) 1; 2; 5; 6

**IIa** none

**IIb** [2]  $P4_2 2_1 2$  ( $\mathbf{c}' = 2\mathbf{c}$ ) (96); [2]  $P4_1 2_1 2$  ( $\mathbf{c}' = 2\mathbf{c}$ ) (92)

**Maximal isomorphic subgroups of lowest index**

**IIc** [3]  $P4_2 2_1 2$  ( $\mathbf{c}' = 3\mathbf{c}$ ) (94); [9]  $P4_2 2_1 2$  ( $\mathbf{a}' = 3\mathbf{a}, \mathbf{b}' = 3\mathbf{b}$ ) (94)

**Minimal non-isomorphic supergroups**

**I** [2]  $P4_2/mbc$  (135); [2]  $P4_2/mnm$  (136); [2]  $P4_2/nmc$  (137); [2]  $P4_2/ncm$  (138)

**II** [2]  $C4_2 22$  ( $P4_2 22, 93$ ); [2]  $I4 22$  (97); [2]  $P4_2 2_1 2$  ( $\mathbf{c}' = \frac{1}{2}\mathbf{c}$ ) (90)