

$P4_2 2_1 2$

$D_4^6$

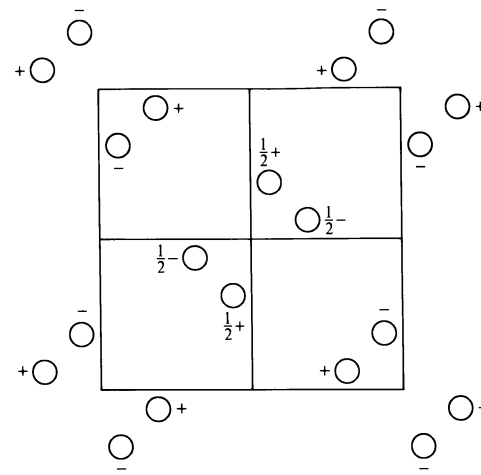
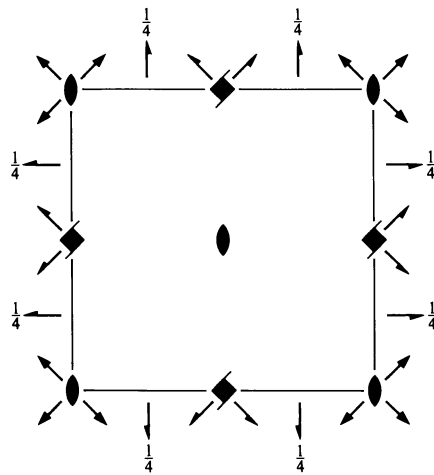
422

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
<b>General:</b>						
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) $\bar{y}, \bar{x}, \bar{z}$	$00l: l = 2n$ $hk0: h = 2n$
<b>Special: as above, plus</b>						
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  $x, x, 0$