

$I4/m$

$C_{4h}^5$

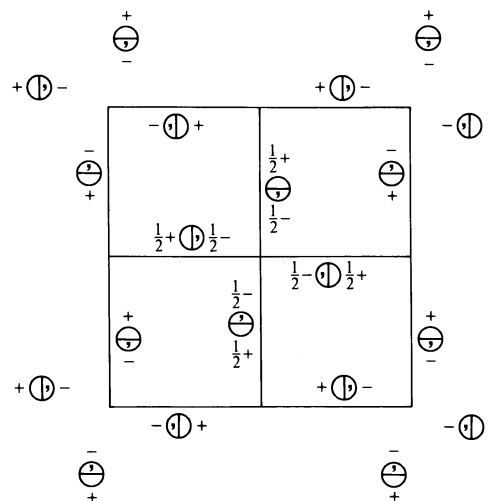
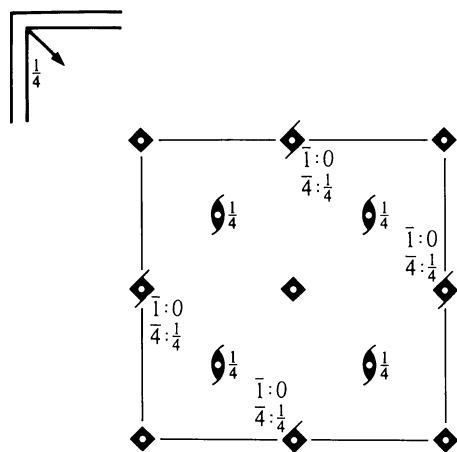
$4/m$

Tetragonal

No. 87

$I4/m$

Patterson symmetry  $I4/m$



**Origin** at centre ( $4/m$ )

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

**Symmetry operations**

For  $(0,0,0)+$  set

- |                       |                 |                                  |                                  |
|-----------------------|-----------------|----------------------------------|----------------------------------|
| (1) 1                 | (2) $2 \ 0,0,z$ | (3) $4^+ \ 0,0,z$                | (4) $4^- \ 0,0,z$                |
| (5) $\bar{1} \ 0,0,0$ | (6) $m \ x,y,0$ | (7) $\bar{4}^+ \ 0,0,z; \ 0,0,0$ | (8) $\bar{4}^- \ 0,0,z; \ 0,0,0$ |

For  $(\frac{1}{2}, \frac{1}{2}, \frac{1}{2})+$  set

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

**Generators selected** (1);  $t(1,0,0)$ ;  $t(0,1,0)$ ;  $t(0,0,1)$ ;  $t(\frac{1}{2}, \frac{1}{2}, \frac{1}{2})$ ; (2); (3); (5)

**Positions**

Multiplicity,  
Wyckoff letter,  
Site symmetry

Coordinates

$(0,0,0)+ (\frac{1}{2}, \frac{1}{2}, \frac{1}{2})+$

Reflection conditions

General:

16 *i* 1 (1)  $x, y, z$  (2)  $\bar{x}, \bar{y}, z$  (3)  $\bar{y}, x, z$  (4)  $y, \bar{x}, z$   
(5)  $\bar{x}, \bar{y}, \bar{z}$  (6)  $x, y, \bar{z}$  (7)  $y, \bar{x}, \bar{z}$  (8)  $\bar{y}, x, \bar{z}$

$hkl: h+k+l=2n$

$hk0: h+k=2n$

$0kl: k+l=2n$

$hhl: l=2n$

$00l: l=2n$

$h00: h=2n$

Special: as above, plus

no extra conditions

$hkl: l=2n$

$hkl: k, l=2n$

no extra conditions

$hkl: l=2n$

$hkl: l=2n$

no extra conditions

no extra conditions

8 *h*  $m..$   $x, y, 0$   $\bar{x}, \bar{y}, 0$   $\bar{y}, x, 0$   $y, \bar{x}, 0$

8 *g*  $2..$   $0, \frac{1}{2}, z$   $\frac{1}{2}, 0, z$   $0, \frac{1}{2}, \bar{z}$   $\frac{1}{2}, 0, \bar{z}$

8 *f*  $\bar{1}$   $\frac{1}{4}, \frac{1}{4}, \frac{1}{4}$   $\frac{3}{4}, \frac{3}{4}, \frac{1}{4}$   $\frac{3}{4}, \frac{1}{4}, \frac{1}{4}$   $\frac{1}{4}, \frac{3}{4}, \frac{1}{4}$

4 *e*  $4..$   $0, 0, z$   $0, 0, \bar{z}$

4 *d*  $\bar{4}..$   $0, \frac{1}{2}, \frac{1}{4}$   $\frac{1}{2}, 0, \frac{1}{4}$

4 *c*  $2/m..$   $0, \frac{1}{2}, 0$   $\frac{1}{2}, 0, 0$

2 *b*  $4/m..$   $0, 0, \frac{1}{2}$

2 *a*  $4/m..$   $0, 0, 0$

**Symmetry of special projections**

Along  $[001]$   $p4$

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

Origin at  $0, 0, z$

Along  $[100]$   $c2mm$

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

Origin at  $x, 0, 0$

Along  $[110]$   $p2mm$

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

Origin at  $x, x, 0$