

Tetragonal

4

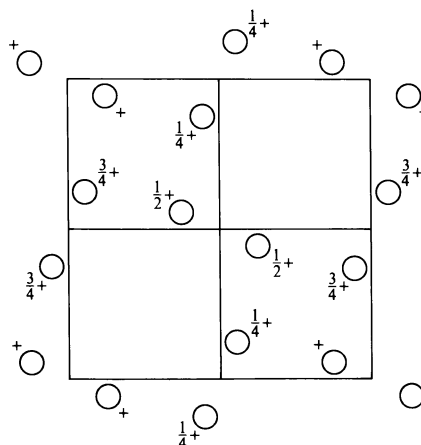
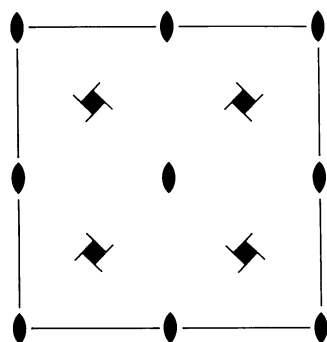
C_4^6

$I4_1$

Patterson symmetry $I4/m$

$I4_1$

No. 80



Origin on 2

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

Symmetry operations

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

- (1) 1 (2) $2(0,0,\frac{1}{2}) \frac{1}{4}, \frac{1}{4}, z$ (3) $4^+(0,0,\frac{1}{4}) -\frac{1}{4}, \frac{1}{4}, z$ (4) $4^-(0,0,\frac{3}{4}) \frac{1}{4}, -\frac{1}{4}, z$

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

- (1) $t(\frac{1}{2}, \frac{1}{2}, \frac{1}{2})$ (2) $2 0,0,z$ (3) $4^+(0,0,\frac{3}{4}) \frac{1}{4}, \frac{1}{4}, z$ (4) $4^-(0,0,\frac{1}{4}) \frac{1}{4}, \frac{1}{4}, z$

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)

Positions

Multiplicity,
Wyckoff letter,
Site symmetry

Coordinates

Reflection conditions

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

General:

8 *b* 1 (1) x,y,z (2) $\bar{x} + \frac{1}{2}, \bar{y} + \frac{1}{2}, z + \frac{1}{2}$ (3) $\bar{y}, x + \frac{1}{2}, z + \frac{1}{4}$ (4) $y + \frac{1}{2}, \bar{x}, z + \frac{3}{4}$

$hkl: h+k+l = 2n$
 $hk0: h+k = 2n$
 $0kl: k+l = 2n$
 $hhl: l = 2n$
 $00l: l = 4n$
 $h00: h = 2n$

Special: as above, plus

4 *a* 2.. $0,0,z$ $0, \frac{1}{2}, z + \frac{1}{4}$

$hkl: l = 2n + 1$
or $2h + l = 4n$

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 $\frac{1}{4}, \frac{1}{4}, z$

Along $[100] c1m1$

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

Origin at $x, 0, 0$

Along $[110] p1m1$

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

Origin at $x, x, 0$