

$I4_1cd$

C_{4v}^{12}

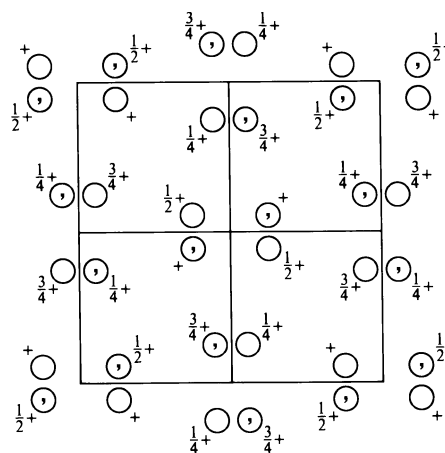
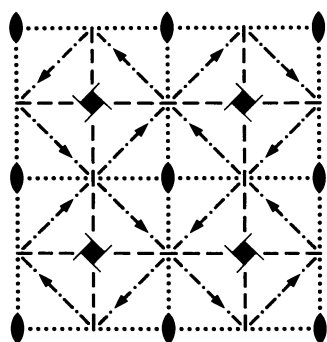
$4mm$

Tetragonal

No. 110

$I4_1cd$

Patterson symmetry $I4/mmm$



Origin on $2c1$

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) $2(0,0,\frac{1}{2}) \frac{1}{4}, \frac{1}{4}, z$
- (3) $4^+(0,0,\frac{1}{4}) -\frac{1}{4}, \frac{1}{4}, z$
- (4) $4^-(0,0,\frac{3}{4}) \frac{1}{4}, -\frac{1}{4}, z$
- (5) $c \ x, 0, z$
- (6) $b \ \frac{1}{4}, y, z$
- (7) $d(-\frac{1}{4}, \frac{1}{4}, \frac{3}{4}) \ x + \frac{1}{4}, \bar{x}, z$
- (8) $d(\frac{1}{4}, \frac{1}{4}, \frac{1}{4}) \ x + \frac{1}{4}, x, z$

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) $4^-(0,0,\frac{1}{4}) \frac{1}{4}, \frac{1}{4}, z$
- (5) $a \ x, \frac{1}{4}, z$
- (6) $c \ 0, y, z$
- (7) $d(\frac{1}{4}, -\frac{1}{4}, \frac{1}{4}) \ x + \frac{1}{4}, \bar{x}, z$
- (8) $d(\frac{1}{4}, \frac{1}{4}, \frac{3}{4}) \ x - \frac{1}{4}, x, z$

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); (5)

Positions

Multiplicity,
Wyckoff letter,
Site symmetry

Coordinates

Reflection conditions

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

General:

- | | | | | | | |
|----|------------|-----------------------------------|---|---|---|-----------------------|
| 16 | <i>b</i> 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) $y + \frac{1}{2}, \bar{x}, z + \frac{3}{4}$ | $hkl: h + k + l = 2n$ |
| | | (5) $x, \bar{y}, z + \frac{1}{2}$ | (6) $\bar{x} + \frac{1}{2}, y + \frac{1}{2}, z$ | (7) $\bar{y}, \bar{x} + \frac{1}{2}, z + \frac{3}{4}$ | (8) $y + \frac{1}{2}, x, z + \frac{1}{4}$ | $hk0: h + k = 2n$ |

- $0kl: k, l = 2n$
- $hhl: 2h + l = 4n$
- $00l: l = 4n$
- $h00: h = 2n$
- $h\bar{h}0: h = 2n$

Special: as above, plus

$hkl: 2h + l = 4n$

Symmetry of special projections

Along $[001] \ p4gm$

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

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

Along $[100] \ p1m1$

$\mathbf{a}' = \frac{1}{2}\mathbf{b} \quad \mathbf{b}' = \frac{1}{2}\mathbf{c}$

Origin at $x, 0, 0$

Along $[110] \ c1m1$

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

Origin at $x, x, 0$