

$I4mm$

C_{4v}^9

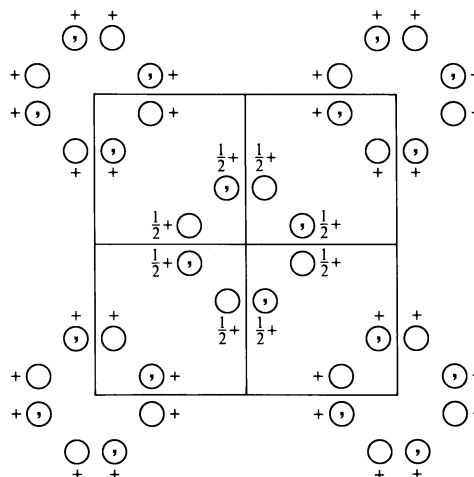
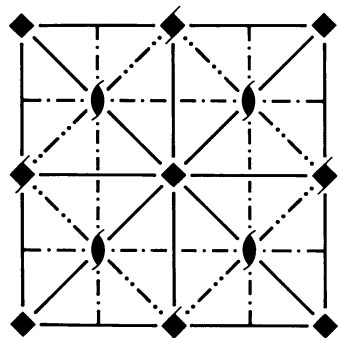
$4mm$

Tetragonal

No. 107

$I4mm$

Patterson symmetry $I4/mmm$



Origin on $4mm$

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

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) $m\ x,0,z$ | (6) $m\ 0,y,z$ | (7) $m\ x,\bar{x},z$ | (8) $m\ x,x,z$ |

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

- | | | | |
|---|---|---|---|
| (1) $t(\frac{1}{2},\frac{1}{2},\frac{1}{2})$ | (2) $2(0,0,\frac{1}{2})\ \frac{1}{4},\frac{1}{4},z$ | (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) $n(\frac{1}{2},0,\frac{1}{2})\ x,\frac{1}{4},z$ | (6) $n(0,\frac{1}{2},\frac{1}{2})\ \frac{1}{4},y,z$ | (7) $c\ x+\frac{1}{2},\bar{x},z$ | (8) $n(\frac{1}{2},\frac{1}{2},\frac{1}{2})\ x,x,z$ |

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>e</i> 1 | (1) x,y,z (5) x,\bar{y},z | (2) \bar{x},\bar{y},z (6) \bar{x},y,z | (3) \bar{y},x,z (7) \bar{y},\bar{x},z | (4) y,\bar{x},z (8) y,x,z | | $hkl : h+k+l=2n$ $hk0 : h+k=2n$ $0kl : k+l=2n$ $hhl : l=2n$ $00l : l=2n$ $h00 : h=2n$ |
| 8 <i>d</i> . <i>m</i> . | $x,0,z$ | $\bar{x},0,z$ | $0,x,z$ | $0,\bar{x},z$ | | Special: as above, plus no extra conditions |
| 8 <i>c</i> . <i>.</i> <i>m</i> | x,x,z | \bar{x},\bar{x},z | \bar{x},x,z | x,\bar{x},z | | no extra conditions |
| 4 <i>b</i> 2 <i>m</i> <i>m</i> . | $0,\frac{1}{2},z$ | $\frac{1}{2},0,z$ | | | | $hkl : l=2n$ |
| 2 <i>a</i> 4 <i>m</i> <i>m</i> | $0,0,z$ | | | | | no extra conditions |

Symmetry of special projections

Along [001] $p4mm$

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

Origin at $0,0,z$

Along [100] $c1m1$

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

Origin at $x,0,0$

Along [110] $p1m1$

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

Origin at $x,x,0$

Maximal non-isomorphic subgroups

| | | |
|------------|---------------------------|--|
| I | [2] $I411$ ($I4$, 79) | (1; 2; 3; 4)+ |
| | [2] $I2m1$ ($Imm2$, 44) | (1; 2; 5; 6)+ |
| | [2] $I21m$ ($Fmm2$, 42) | (1; 2; 7; 8)+ |
| IIa | [2] $P4_2mc$ (105) | 1; 2; 5; 6; (3; 4; 7; 8) + $(\frac{1}{2},\frac{1}{2},\frac{1}{2})$ |
| | [2] $P4nc$ (104) | 1; 2; 3; 4; (5; 6; 7; 8) + $(\frac{1}{2},\frac{1}{2},\frac{1}{2})$ |
| | [2] $P4_2nm$ (102) | 1; 2; 7; 8; (3; 4; 5; 6) + $(\frac{1}{2},\frac{1}{2},\frac{1}{2})$ |
| | [2] $P4mm$ (99) | 1; 2; 3; 4; 5; 6; 7; 8 |
| IIb | none | |

Maximal isomorphic subgroups of lowest index

IIc [3] $I4mm$ ($\mathbf{c}' = 3\mathbf{c}$) (107); [9] $I4mm$ ($\mathbf{a}' = 3\mathbf{a}, \mathbf{b}' = 3\mathbf{b}$) (107)

Minimal non-isomorphic supergroups

| | |
|-----------|---|
| I | [2] $I4/mmm$ (139) |
| II | [2] $C4mm$ ($\mathbf{c}' = \frac{1}{2}\mathbf{c}$) ($P4mm$, 99) |