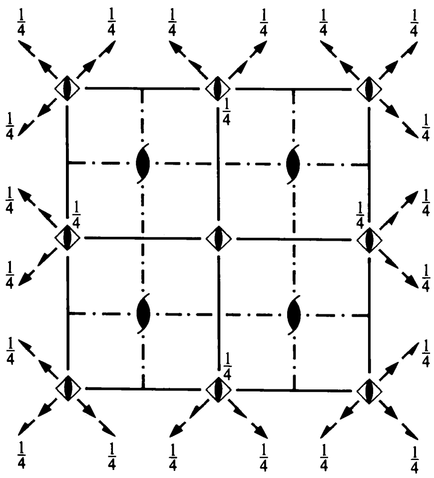
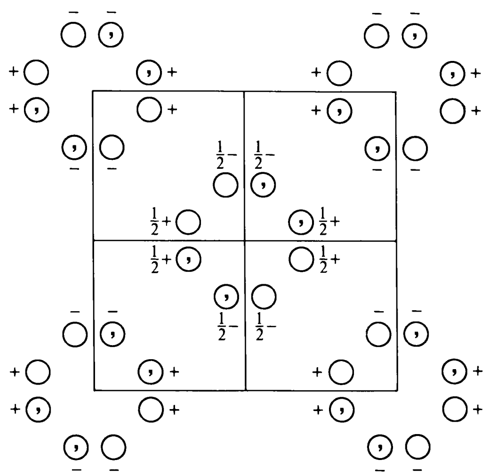
# $I\bar{4}m2$ $D_{2d}^{9}$ $\bar{4}m2$ Tetragonal

No. 119 $I\bar{4}m2$ Patterson symmetry $I4/mmm$





**Origin** at $\bar{4}m2$

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

**Symmetry operations**

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

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

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

**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 | *j* | 1 | (1) $x,y,z$ (5) $x,\bar{y},z$ | (2) $\bar{x},\bar{y},z$ (6) $\bar{x},y,z$ | (3) $y,\bar{x},\bar{z}$ (7) $y,x,\bar{z}$ | (4) $\bar{y},x,\bar{z}$ (8) $\bar{y},\bar{x},\bar{z}$ | $hkl$ : $h+k+l=2n$<br>$hk0$ : $h+k=2n$<br>$0kl$ : $k+l=2n$<br>$hhl$ : $l=2n$<br>$00l$ : $l=2n$<br>$h00$ : $h=2n$ |
| | | | | | | | Special: no extra conditions |
| 8 | *i* | $.m.$ | $x,0,z$ | $\bar{x},0,z$ | $0,\bar{x},\bar{z}$ | $0,x,\bar{z}$ | |
| 8 | *h* | $..2$ | $x,x+\frac{1}{2},\frac{1}{4}$ | $\bar{x},\bar{x}+\frac{1}{2},\frac{1}{4}$ | $x+\frac{1}{2},\bar{x},\frac{3}{4}$ | $\bar{x}+\frac{1}{2},x,\frac{3}{4}$ | |
| 8 | *g* | $..2$ | $x,x,0$ | $\bar{x},\bar{x},0$ | $x,\bar{x},0$ | $\bar{x},x,0$ | |
| 4 | *f* | $2mm.$ | $0,\frac{1}{2},z$ | $\frac{1}{2},0,\bar{z}$ | | | |
| 4 | *e* | $2mm.$ | $0,0,z$ | $0,0,\bar{z}$ | | | |
| 2 | *d* | $\bar{4}m2$ | $0,\frac{1}{2},\frac{3}{4}$ | | | | |
| 2 | *c* | $\bar{4}m2$ | $0,\frac{1}{2},\frac{1}{4}$ | | | | |
| 2 | *b* | $\bar{4}m2$ | $0,0,\frac{1}{2}$ | | | | |
| 2 | *a* | $\bar{4}m2$ | $0,0,0$ | | | | |

## Symmetry of special projections

Along [001] $p4mm$
$\mathbf{a}'=\frac{1}{2}(\mathbf{a}-\mathbf{b})$ $\mathbf{b}'=\frac{1}{2}(\mathbf{a}+\mathbf{b})$
Origin at $0,0,z$

Along [100] $c1m1$
$\mathbf{a}'=\mathbf{b}$ $\mathbf{b}'=\mathbf{c}$
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 $x,x,0$

## Maximal non-isomorphic subgroups

**I** [2] $I\bar{4}11$ ($I\bar{4}$, 82) (1; 2; 3; 4)+
[2] $I2m1$ ($Imm2$, 44) (1; 2; 5; 6)+
[2] $I212$ ($F222$, 22) (1; 2; 7; 8)+

**IIa** [2] $P\bar{4}n2$ (118) 1; 2; 3; 4; (5; 6; 7; 8) + $(\frac{1}{2},\frac{1}{2},\frac{1}{2})$
[2] $P\bar{4}n2$ (118) 1; 2; 7; 8; (3; 4; 5; 6) + $(\frac{1}{2},\frac{1}{2},\frac{1}{2})$
[2] $P\bar{4}m2$ (115) 1; 2; 3; 4; 5; 6; 7; 8
[2] $P\bar{4}m2$ (115) 1; 2; 5; 6; (3; 4; 7; 8) + $(\frac{1}{2},\frac{1}{2},\frac{1}{2})$

**IIb** none

## Maximal isomorphic subgroups of lowest index

**IIc** [3] $I\bar{4}m2$ ($\mathbf{c}'=3\mathbf{c}$) (119); [9] $I\bar{4}m2$ ($\mathbf{a}'=3\mathbf{a},\mathbf{b}'=3\mathbf{b}$) (119)

## Minimal non-isomorphic supergroups

**I** [2] $I4/mmm$ (139); [2] $I4_1/amd$ (141); [3] $F\bar{4}3m$ (216)

**II** [2] $C\bar{4}m2$ ($\mathbf{c}'=\frac{1}{2}\mathbf{c}$) ($P\bar{4}2m$, 111)