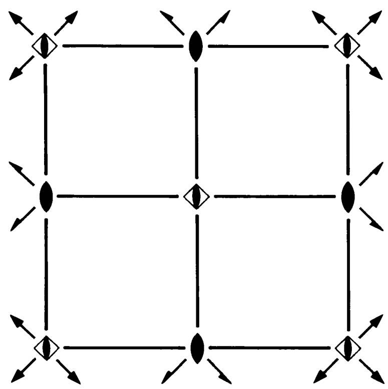
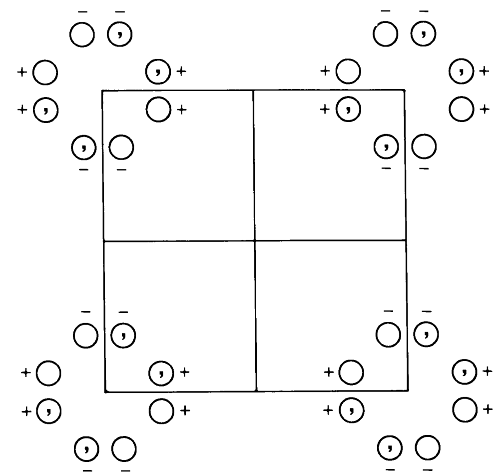
Tetragonal $\bar{4}m2$ $D_{2d}^5$ $P\bar{4}m2$

Patterson symmetry $P4/mmm$ $P\bar{4}m2$ No. 115






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

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

**Symmetry operations**

| | | | |
|---|---|---|---|
| (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 $x,\bar{x},0$ |

**Generators selected** (1); $t(1,0,0)$; $t(0,1,0)$; $t(0,0,1)$; (2); (3); (5)

**Positions**

| Multiplicity, Wyckoff letter, Site symmetry | | | Coordinates | | | | Reflection conditions |
|---|---|---|---|---|---|---|---|
| | | | | | | | General: |
| 8 | $l$ | 1 | (1) $x,y,z$ | (2) $\bar{x},\bar{y},z$ | (3) $y,\bar{x},\bar{z}$ | (4) $\bar{y},x,\bar{z}$ | no conditions |
| | | | (5) $x,\bar{y},z$ | (6) $\bar{x},y,z$ | (7) $y,x,\bar{z}$ | (8) $\bar{y},\bar{x},\bar{z}$ | |
| | | | | | | | Special: |
| 4 | $k$ | $.m.$ | $x,\frac{1}{2},z$ | $\bar{x},\frac{1}{2},z$ | $\frac{1}{2},\bar{x},\bar{z}$ | $\frac{1}{2},x,\bar{z}$ | no extra conditions |
| 4 | $j$ | $.m.$ | $x,0,z$ | $\bar{x},0,z$ | $0,\bar{x},\bar{z}$ | $0,x,\bar{z}$ | no extra conditions |
| 4 | $i$ | $..2$ | $x,x,\frac{1}{2}$ | $\bar{x},\bar{x},\frac{1}{2}$ | $x,\bar{x},\frac{1}{2}$ | $\bar{x},x,\frac{1}{2}$ | no extra conditions |
| 4 | $h$ | $..2$ | $x,x,0$ | $\bar{x},\bar{x},0$ | $x,\bar{x},0$ | $\bar{x},x,0$ | no extra conditions |
| 2 | $g$ | $2mm.$ | $0,\frac{1}{2},z$ | $\frac{1}{2},0,\bar{z}$ | | | $hk0$: $h+k=2n$ |
| 2 | $f$ | $2mm.$ | $\frac{1}{2},\frac{1}{2},z$ | $\frac{1}{2},\frac{1}{2},\bar{z}$ | | | no extra conditions |
| 2 | $e$ | $2mm.$ | $0,0,z$ | $0,0,\bar{z}$ | | | no extra conditions |
| 1 | $d$ | $\bar{4}m2$ | $0,0,\frac{1}{2}$ | | | | no extra conditions |
| 1 | $c$ | $\bar{4}m2$ | $\frac{1}{2},\frac{1}{2},\frac{1}{2}$ | | | | no extra conditions |
| 1 | $b$ | $\bar{4}m2$ | $\frac{1}{2},\frac{1}{2},0$ | | | | no extra conditions |
| 1 | $a$ | $\bar{4}m2$ | $0,0,0$ | | | | no extra conditions |

**Symmetry of special projections**

Along [001] $p4mm$
$\mathbf{a}' = \mathbf{a}$ $\mathbf{b}' = \mathbf{b}$
Origin at $0,0,z$

Along [100] $p1m1$
$\mathbf{a}' = \mathbf{b}$ $\mathbf{b}' = \mathbf{c}$
Origin at $x,0,0$

Along [110] $p2mm$
$\mathbf{a}' = \frac{1}{2}(-\mathbf{a}+\mathbf{b})$ $\mathbf{b}' = \mathbf{c}$
Origin at $x,x,0$