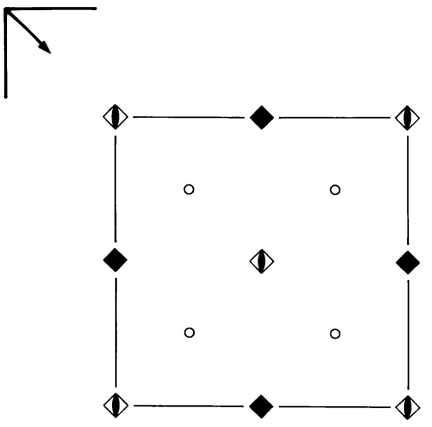
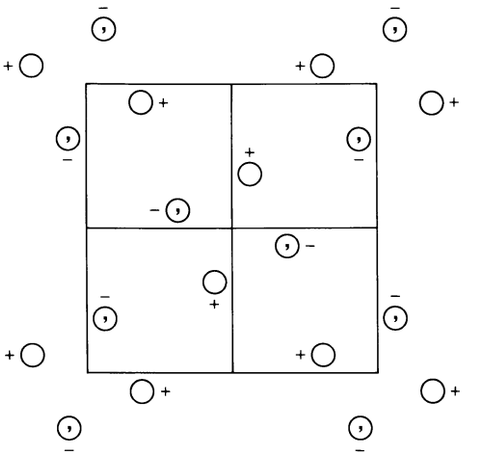
# $P4/n$ $C_{4h}^3$ $4/m$ Tetragonal

No. 85 $P4/n$ Patterson symmetry $P4/m$

ORIGIN CHOICE 1





**Origin** at $\bar{4}$ on $n$, at $-\frac{1}{4},\frac{1}{4},0$ from $\bar{1}$

**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) $4^+$ $0,\frac{1}{2},z$
(4) $4^-$ $\frac{1}{2},0,z$
(5) $\bar{1}$ $\frac{1}{4},\frac{1}{4},0$
(6) $n(\frac{1}{2},\frac{1}{2},0)$ $x,y,0$
(7) $\bar{4}^+$ $0,0,z$; $0,0,0$
(8) $\bar{4}^-$ $0,0,z$; $0,0,0$

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

**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 $0,0,z$

Along [100] $p2mg$
$\mathbf{a}'=\mathbf{b}$ $\mathbf{b}'=\mathbf{c}$
Origin at $x,\frac{1}{4},0$

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

**Maximal non-isomorphic subgroups**

**I** [2] $P\bar{4}$ (81) 1; 2; 7; 8
[2] $P4$ (75) 1; 2; 3; 4
[2] $P2/n$ ($P2/c$, 13) 1; 2; 5; 6

**IIa** none

**IIb** [2] $P4_2/n$ ($\mathbf{c}'=2\mathbf{c}$) (86)

**Maximal isomorphic subgroups of lowest index**

**IIc** [2] $P4/n$ ($\mathbf{c}'=2\mathbf{c}$) (85); [5] $P4/n$ ($\mathbf{a}'=\mathbf{a}+2\mathbf{b},\mathbf{b}'=-2\mathbf{a}+\mathbf{b}$ or $\mathbf{a}'=\mathbf{a}-2\mathbf{b},\mathbf{b}'=2\mathbf{a}+\mathbf{b}$) (85)

**Minimal non-isomorphic supergroups**

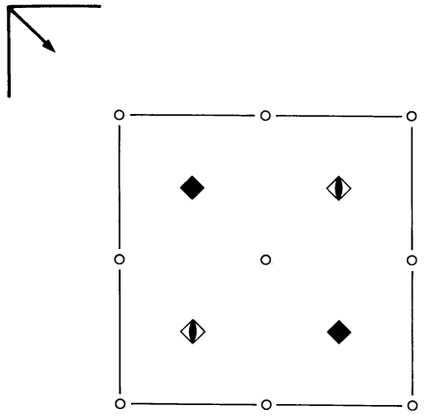
**I** [2] $P4/nbm$ (125); [2] $P4/nnc$ (126); [2] $P4/nmm$ (129); [2] $P4/ncc$ (130)

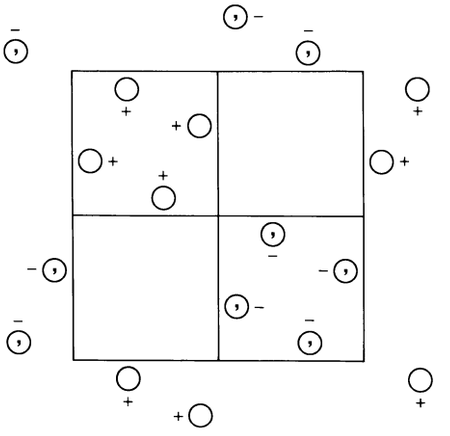
**II** [2] $C4/m$ ($P4/m$, 83); [2] $I4/m$ (87)

# $P4/n$ $C_{4h}^3$ $4/m$ Tetragonal

No. 85 $P4/n$ Patterson symmetry $P4/m$

ORIGIN CHOICE 2





**Origin** at $\bar{1}$ on $n$, at $\frac{1}{4},-\frac{1}{4},0$ from $\bar{4}$

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

**Symmetry operations**

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

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

**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] $p2mg$
$\mathbf{a}' = \mathbf{b}$ $\mathbf{b}' = \mathbf{c}$
Origin at $x,0,0$

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

**Maximal non-isomorphic subgroups**

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**Maximal isomorphic subgroups of lowest index**

**IIc** [2] $P4/n$ ($\mathbf{c}' = 2\mathbf{c}$) (85); [5] $P4/n$ ($\mathbf{a}' = \mathbf{a}+2\mathbf{b}, \mathbf{b}' = -2\mathbf{a}+\mathbf{b}$ or $\mathbf{a}' = \mathbf{a}-2\mathbf{b}, \mathbf{b}' = 2\mathbf{a}+\mathbf{b}$) (85)

**Minimal non-isomorphic supergroups**

**I** [2] $P4/nbm$ (125); [2] $P4/nnc$ (126); [2] $P4/nmm$ (129); [2] $P4/ncc$ (130)

**II** [2] $C4/m$ ($P4/m$, 83); [2] $I4/m$ (87)