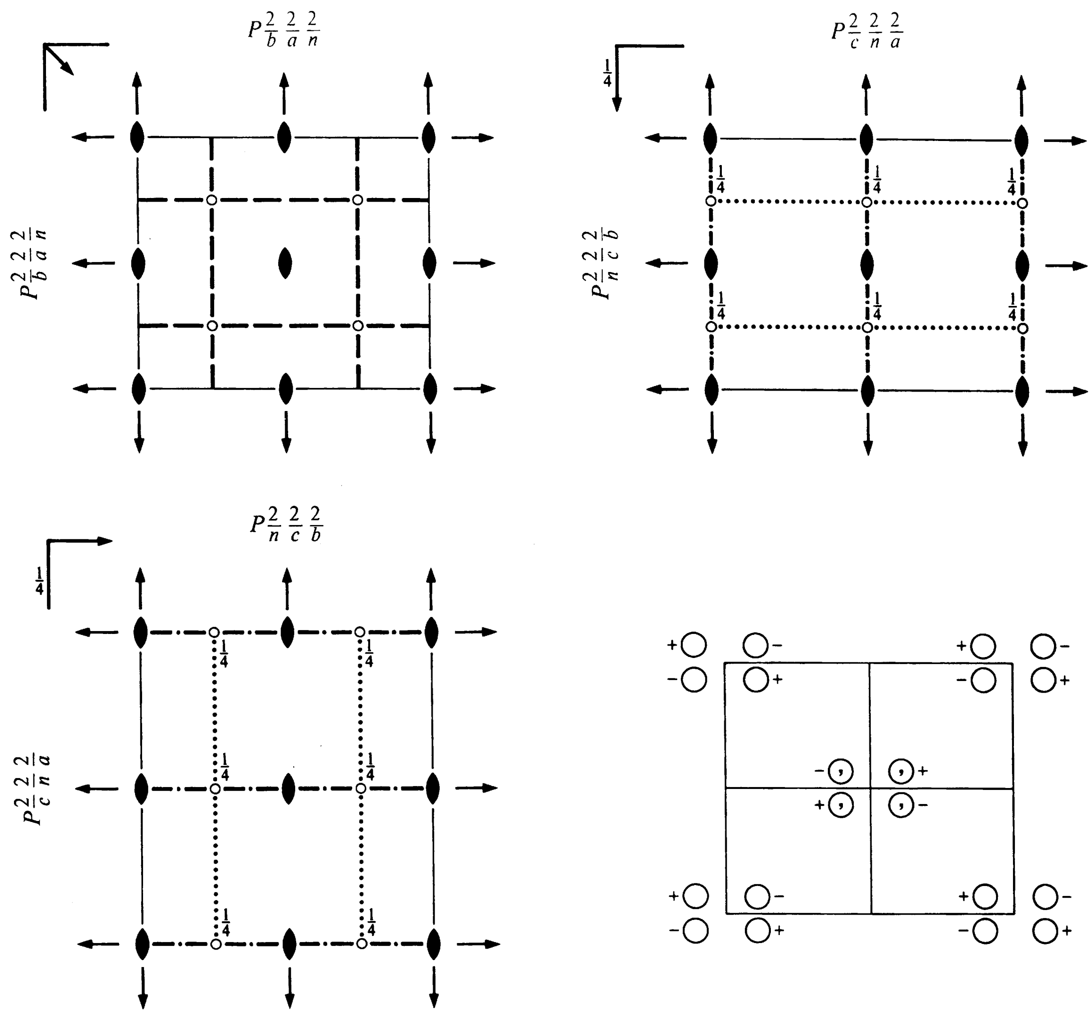
*International Tables for Crystallography* (2006). Vol. A, Space group 50, pp. 270–273.

# *Pban* $D_{2h}^{4}$ *mmm* Orthorhombic

**No. 50** $P\ 2/b\ 2/a\ 2/n$ Patterson symmetry *Pmmm*

ORIGIN CHOICE 1




**Origin** at $222/n$, at $\frac{1}{4},\frac{1}{4},0$ from $\bar{1}$

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

**Symmetry operations**

| | | | |
|---|---|---|---|
| (1) 1 | (2) 2 $0,0,z$ | (3) 2 $0,y,0$ | (4) 2 $x,0,0$ |
| (5) $\bar{1}$ $\frac{1}{4},\frac{1}{4},0$ | (6) $n(\frac{1}{2},\frac{1}{2},0)$ $x,y,0$ | (7) $a$ $x,\frac{1}{4},z$ | (8) $b$ $\frac{1}{4},y,z$ |

**Minimal non-isomorphic supergroups**

**I** [2] $P4/nbm$ (125); [2] $P4_2/nbc$ (133)

**II** [2] $Cmmm$ (65); [2] $Aeaa$ ($Ccce$, 68); [2] $Bbeb$ ($Ccce$, 68); [2] $Ibam$ (72); [2] $Pbmb$ ($\mathbf{a}' = \frac{1}{2}\mathbf{a}$) ($Pccm$, 49); [2] $Pmaa$ ($\mathbf{b}' = \frac{1}{2}\mathbf{b}$) ($Pccm$, 49)

**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 | *m* | 1 | (1) $x,y,z$ <br> (5) $\bar{x}+\frac{1}{2},\bar{y}+\frac{1}{2},\bar{z}$ | (2) $\bar{x},\bar{y},z$ <br> (6) $x+\frac{1}{2},y+\frac{1}{2},\bar{z}$ | (3) $\bar{x},y,\bar{z}$ <br> (7) $x+\frac{1}{2},\bar{y}+\frac{1}{2},z$ | (4) $x,\bar{y},\bar{z}$ <br> (8) $\bar{x}+\frac{1}{2},y+\frac{1}{2},z$ | $0kl$ : $k=2n$ <br> $h0l$ : $h=2n$ <br> $hk0$ : $h+k=2n$ <br> $h00$ : $h=2n$ <br> $0k0$ : $k=2n$ |
| | | | | | | | Special: as above, plus |
| 4 | *l* | . . 2 | $0,\frac{1}{2},z$ | $0,\frac{1}{2},\bar{z}$ | $\frac{1}{2},0,\bar{z}$ | $\frac{1}{2},0,z$ | $hkl$ : $h+k=2n$ |
| 4 | *k* | . . 2 | $0,0,z$ | $0,0,\bar{z}$ | $\frac{1}{2},\frac{1}{2},\bar{z}$ | $\frac{1}{2},\frac{1}{2},z$ | $hkl$ : $h+k=2n$ |
| 4 | *j* | . 2 . | $0,y,\frac{1}{2}$ | $0,\bar{y},\frac{1}{2}$ | $\frac{1}{2},\bar{y}+\frac{1}{2},\frac{1}{2}$ | $\frac{1}{2},y+\frac{1}{2},\frac{1}{2}$ | $hkl$ : $h+k=2n$ |
| 4 | *i* | . 2 . | $0,y,0$ | $0,\bar{y},0$ | $\frac{1}{2},\bar{y}+\frac{1}{2},0$ | $\frac{1}{2},y+\frac{1}{2},0$ | $hkl$ : $h+k=2n$ |
| 4 | *h* | 2 . . | $x,0,\frac{1}{2}$ | $\bar{x},0,\frac{1}{2}$ | $\bar{x}+\frac{1}{2},\frac{1}{2},\frac{1}{2}$ | $x+\frac{1}{2},\frac{1}{2},\frac{1}{2}$ | $hkl$ : $h+k=2n$ |
| 4 | *g* | 2 . . | $x,0,0$ | $\bar{x},0,0$ | $\bar{x}+\frac{1}{2},\frac{1}{2},0$ | $x+\frac{1}{2},\frac{1}{2},0$ | $hkl$ : $h+k=2n$ |
| 4 | *f* | $\bar{1}$ | $\frac{1}{4},\frac{1}{4},\frac{1}{2}$ | $\frac{3}{4},\frac{3}{4},\frac{1}{2}$ | $\frac{3}{4},\frac{1}{4},\frac{1}{2}$ | $\frac{1}{4},\frac{3}{4},\frac{1}{2}$ | $hkl$ : $h,k=2n$ |
| 4 | *e* | $\bar{1}$ | $\frac{1}{4},\frac{1}{4},0$ | $\frac{3}{4},\frac{3}{4},0$ | $\frac{3}{4},\frac{1}{4},0$ | $\frac{1}{4},\frac{3}{4},0$ | $hkl$ : $h,k=2n$ |
| 2 | *d* | 2 2 2 | $0,0,\frac{1}{2}$ | $\frac{1}{2},\frac{1}{2},\frac{1}{2}$ | | | $hkl$ : $h+k=2n$ |
| 2 | *c* | 2 2 2 | $\frac{1}{2},0,\frac{1}{2}$ | $0,\frac{1}{2},\frac{1}{2}$ | | | $hkl$ : $h+k=2n$ |
| 2 | *b* | 2 2 2 | $\frac{1}{2},0,0$ | $0,\frac{1}{2},0$ | | | $hkl$ : $h+k=2n$ |
| 2 | *a* | 2 2 2 | $0,0,0$ | $\frac{1}{2},\frac{1}{2},0$ | | | $hkl$ : $h+k=2n$ |

**Symmetry of special projections**

Along [001] $c2mm$
$\mathbf{a}'=\mathbf{a}$ $\mathbf{b}'=\mathbf{b}$
Origin at $0,0,z$

Along [100] $p2mm$
$\mathbf{a}'=\frac{1}{2}\mathbf{b}$ $\mathbf{b}'=\mathbf{c}$
Origin at $x,0,0$

Along [010] $p2mm$
$\mathbf{a}'=\mathbf{c}$ $\mathbf{b}'=\frac{1}{2}\mathbf{a}$
Origin at $0,y,0$

**Maximal non-isomorphic subgroups**

| | | |
|---|---|---|
| **I** | [2] $Pba2$ (32) | 1; 2; 7; 8 |
| | [2] $Pb2n$ ($Pnc2$, 30) | 1; 3; 6; 8 |
| | [2] $P2an$ ($Pnc2$, 30) | 1; 4; 6; 7 |
| | [2] $P222$ (16) | 1; 2; 3; 4 |
| | [2] $P112/n$ ($P2/c$, 13) | 1; 2; 5; 6 |
| | [2] $P12/a1$ ($P2/c$, 13) | 1; 3; 5; 7 |
| | [2] $P2/b11$ ($P2/c$, 13) | 1; 4; 5; 8 |

**IIa** none

**IIb** [2] $Pnan$ ($\mathbf{c}'=2\mathbf{c}$) ($Pnna$, 52); [2] $Pbnn$ ($\mathbf{c}'=2\mathbf{c}$) ($Pnna$, 52); [2] $Pnnn$ ($\mathbf{c}'=2\mathbf{c}$) (48)

**Maximal isomorphic subgroups of lowest index**

**IIc** [2] $Pban$ ($\mathbf{c}'=2\mathbf{c}$) (50); [3] $Pban$ ($\mathbf{a}'=3\mathbf{a}$ or $\mathbf{b}'=3\mathbf{b}$) (50)

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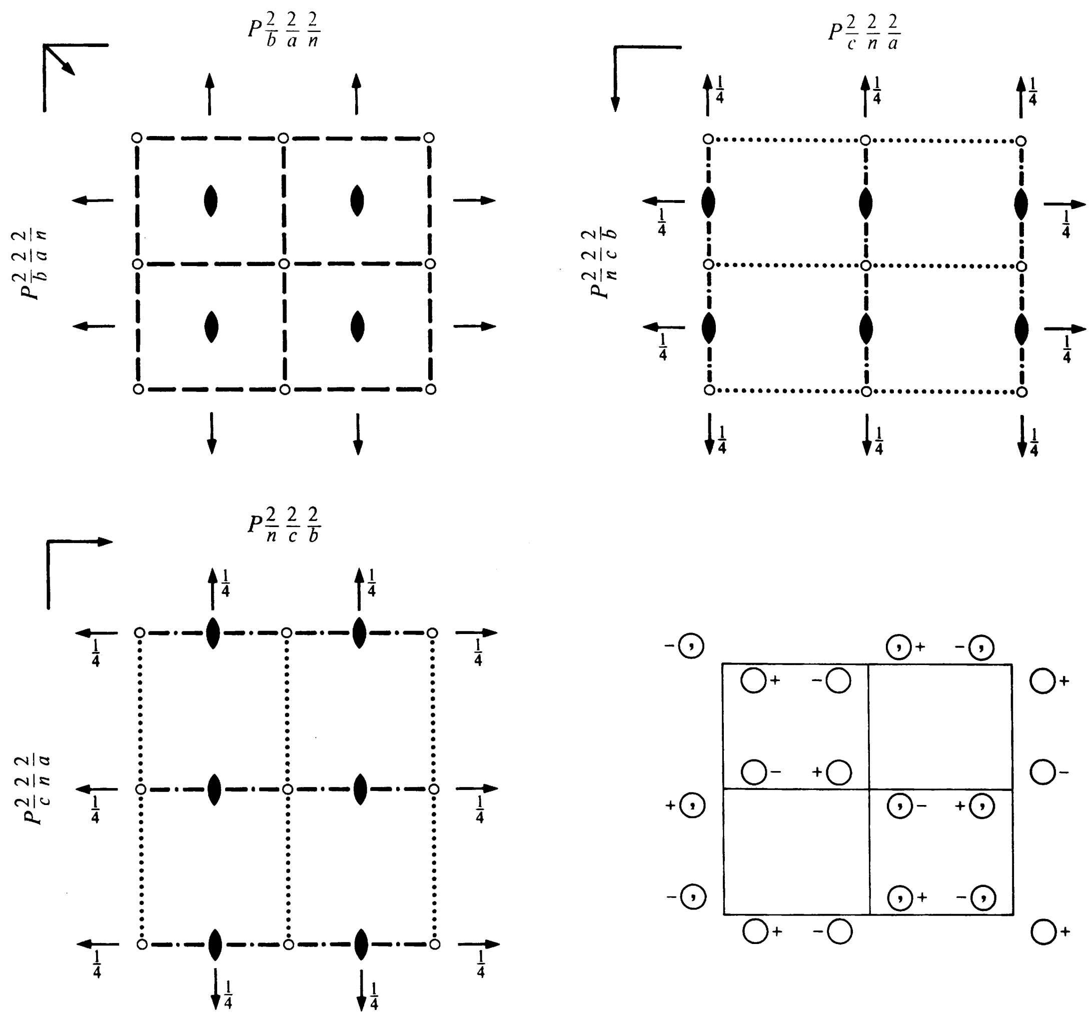
# *Pban* $D_{2h}^{4}$ *mmm* Orthorhombic

No. 50 $P\ 2/b\ 2/a\ 2/n$ Patterson symmetry *Pmmm*

ORIGIN CHOICE 2



**Origin** at $\bar{1}$ at *ban*, at $-\frac{1}{4},-\frac{1}{4},0$ from 222

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

**Symmetry operations**

| | | | |
|---|---|---|---|
| (1) 1 | (2) 2 $\frac{1}{4},\frac{1}{4},z$ | (3) 2 $\frac{1}{4},y,0$ | (4) 2 $x,\frac{1}{4},0$ |
| (5) $\bar{1}$ 0,0,0 | (6) $n(\frac{1}{2},\frac{1}{2},0)$ $x,y,0$ | (7) $a$ $x,0,z$ | (8) $b$ $0,y,z$ |

**Minimal non-isomorphic supergroups**

**I** [2] $P4/nbm$ (125); [2] $P4_2/nbc$ (133)

**II** [2] $Cmmm$ (65); [2] $Aeaa$ ($Ccce$, 68); [2] $Bbeb$ ($Ccce$, 68); [2] $Ibam$ (72); [2] $Pbmb$ ($\mathbf{a}' = \frac{1}{2}\mathbf{a}$) ($Pccm$, 49); [2] $Pmaa$ ($\mathbf{b}' = \frac{1}{2}\mathbf{b}$) ($Pccm$, 49)

**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 | *m* | 1 | (1) $x,y,z$ (5) $\bar{x},\bar{y},\bar{z}$ | (2) $\bar{x}+\frac{1}{2},\bar{y}+\frac{1}{2},z$ (6) $x+\frac{1}{2},y+\frac{1}{2},\bar{z}$ | (3) $\bar{x}+\frac{1}{2},y,\bar{z}$ (7) $x+\frac{1}{2},\bar{y},z$ | (4) $x,\bar{y}+\frac{1}{2},\bar{z}$ (8) $\bar{x},y+\frac{1}{2},z$ | $0kl$ : $k=2n$<br>$h0l$ : $h=2n$<br>$hk0$ : $h+k=2n$<br>$h00$ : $h=2n$<br>$0k0$ : $k=2n$ |
| | | | | | | | Special: as above, plus |
| 4 | *l* | . . 2 | $\frac{1}{4},\frac{3}{4},z$ | $\frac{1}{4},\frac{3}{4},\bar{z}$ | $\frac{3}{4},\frac{1}{4},\bar{z}$ | $\frac{3}{4},\frac{1}{4},z$ | $hkl$ : $h+k=2n$ |
| 4 | *k* | . . 2 | $\frac{1}{4},\frac{1}{4},z$ | $\frac{1}{4},\frac{1}{4},\bar{z}$ | $\frac{3}{4},\frac{3}{4},\bar{z}$ | $\frac{3}{4},\frac{3}{4},z$ | $hkl$ : $h+k=2n$ |
| 4 | *j* | . 2 . | $\frac{1}{4},y,\frac{1}{2}$ | $\frac{1}{4},\bar{y}+\frac{1}{2},\frac{1}{2}$ | $\frac{3}{4},\bar{y},\frac{1}{2}$ | $\frac{3}{4},y+\frac{1}{2},\frac{1}{2}$ | $hkl$ : $h+k=2n$ |
| 4 | *i* | . 2 . | $\frac{1}{4},y,0$ | $\frac{1}{4},\bar{y}+\frac{1}{2},0$ | $\frac{3}{4},\bar{y},0$ | $\frac{3}{4},y+\frac{1}{2},0$ | $hkl$ : $h+k=2n$ |
| 4 | *h* | 2 . . | $x,\frac{1}{4},\frac{1}{2}$ | $\bar{x}+\frac{1}{2},\frac{1}{4},\frac{1}{2}$ | $\bar{x},\frac{3}{4},\frac{1}{2}$ | $x+\frac{1}{2},\frac{3}{4},\frac{1}{2}$ | $hkl$ : $h+k=2n$ |
| 4 | *g* | 2 . . | $x,\frac{1}{4},0$ | $\bar{x}+\frac{1}{2},\frac{1}{4},0$ | $\bar{x},\frac{3}{4},0$ | $x+\frac{1}{2},\frac{3}{4},0$ | $hkl$ : $h+k=2n$ |
| 4 | *f* | $\bar{1}$ | $0,0,\frac{1}{2}$ | $\frac{1}{2},\frac{1}{2},\frac{1}{2}$ | $\frac{1}{2},0,\frac{1}{2}$ | $0,\frac{1}{2},\frac{1}{2}$ | $hkl$ : $h,k=2n$ |
| 4 | *e* | $\bar{1}$ | $0,0,0$ | $\frac{1}{2},\frac{1}{2},0$ | $\frac{1}{2},0,0$ | $0,\frac{1}{2},0$ | $hkl$ : $h,k=2n$ |
| 2 | *d* | 2 2 2 | $\frac{1}{4},\frac{1}{4},\frac{1}{2}$ | $\frac{3}{4},\frac{3}{4},\frac{1}{2}$ | | | $hkl$ : $h+k=2n$ |
| 2 | *c* | 2 2 2 | $\frac{3}{4},\frac{1}{4},\frac{1}{2}$ | $\frac{1}{4},\frac{3}{4},\frac{1}{2}$ | | | $hkl$ : $h+k=2n$ |
| 2 | *b* | 2 2 2 | $\frac{3}{4},\frac{1}{4},0$ | $\frac{1}{4},\frac{3}{4},0$ | | | $hkl$ : $h+k=2n$ |
| 2 | *a* | 2 2 2 | $\frac{1}{4},\frac{1}{4},0$ | $\frac{3}{4},\frac{3}{4},0$ | | | $hkl$ : $h+k=2n$ |

### Symmetry of special projections

Along [001] $c2mm$
$\mathbf{a}'=\mathbf{a}$ $\mathbf{b}'=\mathbf{b}$
Origin at $\frac{1}{4},\frac{1}{4},z$

Along [100] $p2mm$
$\mathbf{a}'=\frac{1}{2}\mathbf{b}$ $\mathbf{b}'=\mathbf{c}$
Origin at $x,0,0$

Along [010] $p2mm$
$\mathbf{a}'=\mathbf{c}$ $\mathbf{b}'=\frac{1}{2}\mathbf{a}$
Origin at $0,y,0$

### Maximal non-isomorphic subgroups

**I** [2] $Pba2$ (32) 1; 2; 7; 8
[2] $Pb2n$ ($Pnc2$, 30) 1; 3; 6; 8
[2] $P2an$ ($Pnc2$, 30) 1; 4; 6; 7
[2] $P222$ (16) 1; 2; 3; 4
[2] $P112/n$ ($P2/c$, 13) 1; 2; 5; 6
[2] $P12/a1$ ($P2/c$, 13) 1; 3; 5; 7
[2] $P2/b11$ ($P2/c$, 13) 1; 4; 5; 8

**IIa** none

**IIb** [2] $Pnan$ ($\mathbf{c}'=2\mathbf{c}$) ($Pnna$, 52); [2] $Pbnn$ ($\mathbf{c}'=2\mathbf{c}$) ($Pnna$, 52); [2] $Pnnn$ ($\mathbf{c}'=2\mathbf{c}$) (48)

### Maximal isomorphic subgroups of lowest index

**IIc** [2] $Pban$ ($\mathbf{c}'=2\mathbf{c}$) (50); [3] $Pban$ ($\mathbf{a}'=3\mathbf{a}$ or $\mathbf{b}'=3\mathbf{b}$) (50)

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