

$P2/m$

C_{2h}^1

$2/m$

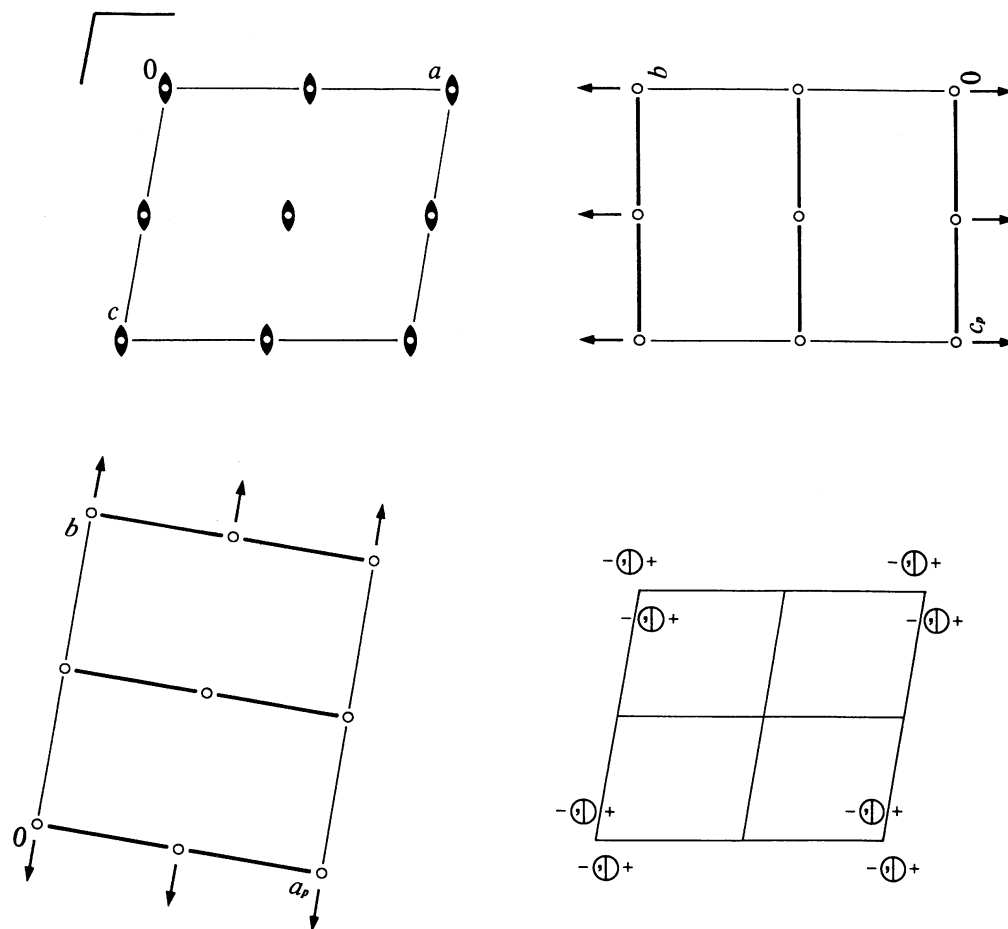
Monoclinic

No. 10

$P12/m1$

Patterson symmetry $P12/m1$

UNIQUE AXIS b



Origin at centre ($2/m$)

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

Symmetry operations

- (1) 1 (2) $2 \ 0,y,0$ (3) $\bar{1} \ 0,0,0$ (4) $m \ x,0,z$

Maximal isomorphic subgroups of lowest index

IIc $[2] P12/m1 (b' = 2b) (P2/m, 10); [2] P12/m1 (c' = 2c \text{ or } a' = 2a \text{ or } a' = a + c, c' = -a + c) (P2/m, 10)$

Minimal non-isomorphic supergroups

I $[2] Pmmm (47); [2] Pccm (49); [2] Pmma (51); [2] Pmna (53); [2] Pbam (55); [2] Pnmm (58); [2] Cmmm (65); [2] Cccm (66); [2] P4/m (83); [2] P4_2/m (84); [3] P6/m (175)$

II $[2] C12/m1 (C2/m, 12); [2] A12/m1 (C2/m, 12); [2] I12/m1 (C2/m, 12)$

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

Positions

| Multiplicity, Wyckoff letter, Site symmetry | | Coordinates | | | | Reflection conditions |
|---|-------------------|---|-------------------------------------|---------------------------------|---------------------|---|
| 4 | <i>o</i> 1 | (1) x, y, z | (2) \bar{x}, y, \bar{z} | (3) $\bar{x}, \bar{y}, \bar{z}$ | (4) x, \bar{y}, z | General: no conditions Special: no extra conditions |
| 2 | <i>n</i> <i>m</i> | $x, \frac{1}{2}, z$ | $\bar{x}, \frac{1}{2}, \bar{z}$ | | | |
| 2 | <i>m</i> <i>m</i> | $x, 0, z$ | $\bar{x}, 0, \bar{z}$ | | | |
| 2 | <i>l</i> 2 | $\frac{1}{2}, y, \frac{1}{2}$ | $\frac{1}{2}, \bar{y}, \frac{1}{2}$ | | | |
| 2 | <i>k</i> 2 | $0, y, \frac{1}{2}$ | $0, \bar{y}, \frac{1}{2}$ | | | |
| 2 | <i>j</i> 2 | $\frac{1}{2}, y, 0$ | $\frac{1}{2}, \bar{y}, 0$ | | | |
| 2 | <i>i</i> 2 | $0, y, 0$ | $0, \bar{y}, 0$ | | | |
| 1 | <i>h</i> $2/m$ | $\frac{1}{2}, \frac{1}{2}, \frac{1}{2}$ | | | | |
| 1 | <i>g</i> $2/m$ | $\frac{1}{2}, 0, \frac{1}{2}$ | | | | |
| 1 | <i>f</i> $2/m$ | $0, \frac{1}{2}, \frac{1}{2}$ | | | | |
| 1 | <i>e</i> $2/m$ | $\frac{1}{2}, \frac{1}{2}, 0$ | | | | |
| 1 | <i>d</i> $2/m$ | $\frac{1}{2}, 0, 0$ | | | | |
| 1 | <i>c</i> $2/m$ | $0, 0, \frac{1}{2}$ | | | | |
| 1 | <i>b</i> $2/m$ | $0, \frac{1}{2}, 0$ | | | | |
| 1 | <i>a</i> $2/m$ | $0, 0, 0$ | | | | |

Symmetry of special projections

Along [001] $p2mm$

$\mathbf{a}' = \mathbf{a}_p$ $\mathbf{b}' = \mathbf{b}$

Origin at 0, 0, z

Along [100] $p2mm$

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

Origin at $x, 0, 0$

Along [010] $p2$

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

Origin at 0, $y, 0$

Maximal non-isomorphic subgroups

I [2] $P1m1$ (Pm , 6) 1; 4
 [2] $P121$ ($P2$, 3) 1; 2
 [2] $P\bar{1}$ (2) 1; 3

IIa none

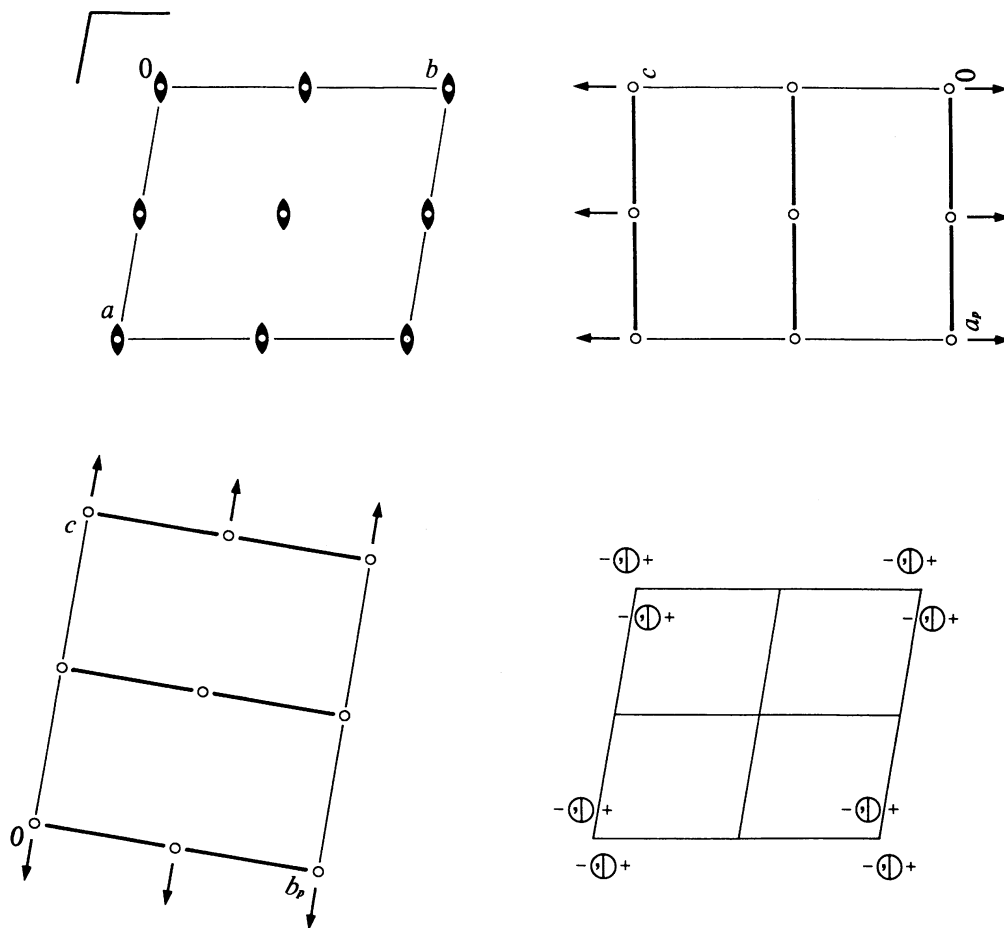
IIb [2] $P12_1/m1$ ($\mathbf{b}' = 2\mathbf{b}$) ($P2_1/m$, 11); [2] $P12/c1$ ($\mathbf{c}' = 2\mathbf{c}$) ($P2/c$, 13); [2] $P12/a1$ ($\mathbf{a}' = 2\mathbf{a}$) ($P2/c$, 13);
 [2] $B12/e1$ ($\mathbf{a}' = 2\mathbf{a}, \mathbf{c}' = 2\mathbf{c}$) ($P2/c$, 13); [2] $C12/m1$ ($\mathbf{a}' = 2\mathbf{a}, \mathbf{b}' = 2\mathbf{b}$) ($C2/m$, 12); [2] $A12/m1$ ($\mathbf{b}' = 2\mathbf{b}, \mathbf{c}' = 2\mathbf{c}$) ($C2/m$, 12);
 [2] $F12/m1$ ($\mathbf{a}' = 2\mathbf{a}, \mathbf{b}' = 2\mathbf{b}, \mathbf{c}' = 2\mathbf{c}$) ($C2/m$, 12)

(Continued on preceding page)

$P2/m$ C_{2h}^1 $2/m$

Monoclinic

No. 10

 $P112/m$ Patterson symmetry $P112/m$ UNIQUE AXIS c **Origin** at centre ($2/m$)**Asymmetric unit** $0 \leq x \leq 1; 0 \leq y \leq \frac{1}{2}; 0 \leq z \leq \frac{1}{2}$ **Symmetry operations**(1) 1 (2) $2 \ 0,0,z$ (3) $\bar{1} \ 0,0,0$ (4) $m \ x,y,0$ **Maximal isomorphic subgroups of lowest index****IIc** $[2] P112/m (c' = 2c) (P2/m, 10); [2] P112/m (a' = 2a \text{ or } b' = 2b \text{ or } a' = a - b, b' = a + b) (P2/m, 10)$ **Minimal non-isomorphic supergroups****I** $[2] Pmmm (47); [2] Pccm (49); [2] Pmma (51); [2] Pmna (53); [2] Pbam (55); [2] Pnnm (58); [2] Cmmm (65); [2] Cccm (66); [2] P4/m (83); [2] P4_2/m (84); [3] P6/m (175)$ **II** $[2] A112/m (C2/m, 12); [2] B112/m (C2/m, 12); [2] I112/m (C2/m, 12)$

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

Positions

| Multiplicity, Wyckoff letter, Site symmetry | Coordinates | | | | Reflection conditions |
|---|---|-------------------------------------|---------------------------------|---------------------|---|
| 4 <i>o</i> 1 | (1) x, y, z | (2) \bar{x}, \bar{y}, z | (3) $\bar{x}, \bar{y}, \bar{z}$ | (4) x, y, \bar{z} | General: no conditions Special: no extra conditions |
| 2 <i>n</i> <i>m</i> | $x, y, \frac{1}{2}$ | $\bar{x}, \bar{y}, \frac{1}{2}$ | | | |
| 2 <i>m</i> <i>m</i> | $x, y, 0$ | $\bar{x}, \bar{y}, 0$ | | | |
| 2 <i>l</i> 2 | $\frac{1}{2}, \frac{1}{2}, z$ | $\frac{1}{2}, \frac{1}{2}, \bar{z}$ | | | |
| 2 <i>k</i> 2 | $\frac{1}{2}, 0, z$ | $\frac{1}{2}, 0, \bar{z}$ | | | |
| 2 <i>j</i> 2 | $0, \frac{1}{2}, z$ | $0, \frac{1}{2}, \bar{z}$ | | | |
| 2 <i>i</i> 2 | $0, 0, z$ | $0, 0, \bar{z}$ | | | |
| 1 <i>h</i> $2/m$ | $\frac{1}{2}, \frac{1}{2}, \frac{1}{2}$ | | | | |
| 1 <i>g</i> $2/m$ | $\frac{1}{2}, \frac{1}{2}, 0$ | | | | |
| 1 <i>f</i> $2/m$ | $\frac{1}{2}, 0, \frac{1}{2}$ | | | | |
| 1 <i>e</i> $2/m$ | $0, \frac{1}{2}, \frac{1}{2}$ | | | | |
| 1 <i>d</i> $2/m$ | $0, \frac{1}{2}, 0$ | | | | |
| 1 <i>c</i> $2/m$ | $\frac{1}{2}, 0, 0$ | | | | |
| 1 <i>b</i> $2/m$ | $0, 0, \frac{1}{2}$ | | | | |
| 1 <i>a</i> $2/m$ | $0, 0, 0$ | | | | |

Symmetry of special projections

Along [001] $p2$
 $\mathbf{a}' = \mathbf{a}$ $\mathbf{b}' = \mathbf{b}$
 Origin at $0, 0, z$

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

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

Maximal non-isomorphic subgroups

I [2] $P11m$ (Pm , 6) 1; 4
 [2] $P112$ ($P2$, 3) 1; 2
 [2] $P\bar{1}$ (2) 1; 3

IIa none

IIb [2] $P112_1/m$ ($\mathbf{c}' = 2\mathbf{c}$) ($P2_1/m$, 11); [2] $P112/a$ ($\mathbf{a}' = 2\mathbf{a}$) ($P2/c$, 13); [2] $P112/b$ ($\mathbf{b}' = 2\mathbf{b}$) ($P2/c$, 13);
 [2] $C112/e$ ($\mathbf{a}' = 2\mathbf{a}, \mathbf{b}' = 2\mathbf{b}$) ($P2/c$, 13); [2] $A112/m$ ($\mathbf{b}' = 2\mathbf{b}, \mathbf{c}' = 2\mathbf{c}$) ($C2/m$, 12); [2] $B112/m$ ($\mathbf{a}' = 2\mathbf{a}, \mathbf{c}' = 2\mathbf{c}$) ($C2/m$, 12);
 [2] $F112/m$ ($\mathbf{a}' = 2\mathbf{a}, \mathbf{b}' = 2\mathbf{b}, \mathbf{c}' = 2\mathbf{c}$) ($C2/m$, 12)

(Continued on preceding page)