

$P2_1$

$C_2^2$

2

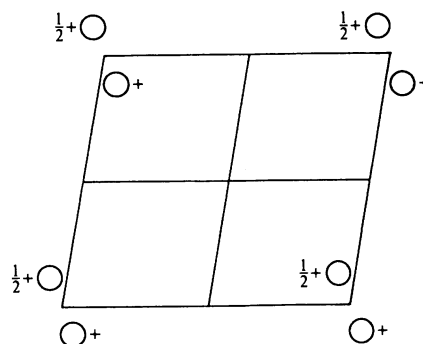
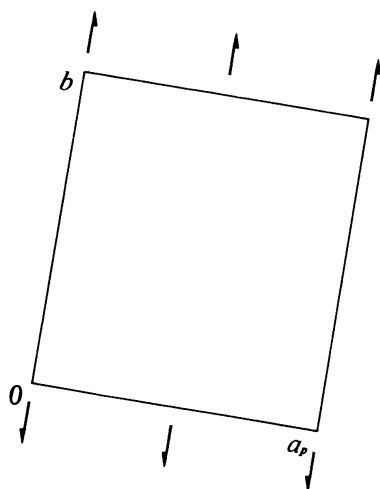
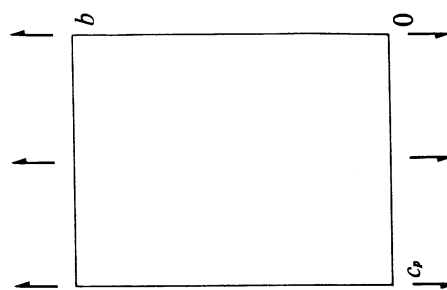
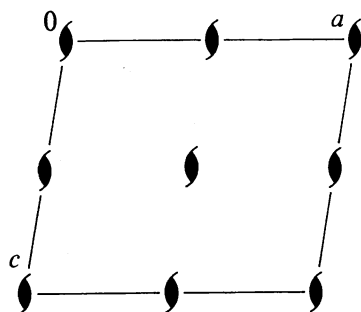
Monoclinic

No. 4

$P12_11$

Patterson symmetry  $P12/m1$

UNIQUE AXIS  $b$



Origin on  $2_1$

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

Symmetry operations

(1) 1 (2)  $2(0, \frac{1}{2}, 0) 0, y, 0$

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

**Positions**

| Multiplicity,<br>Wyckoff letter,<br>Site symmetry | Coordinates   | Reflection conditions |
|---|---|-----------------------|
|   |   | General:              |
| 2 $a$ 1   | (1) $x, y, z$ (2) $\bar{x}, y + \frac{1}{2}, \bar{z}$ | $0k0 : k = 2n$        |

**Symmetry of special projections**

|  |  |  |
|--|--|--|
| Along [001] $p1g1$<br>$\mathbf{a}' = \mathbf{a}_p$ $\mathbf{b}' = \mathbf{b}$<br>Origin at $0, 0, z$ | Along [100] $p11g$<br>$\mathbf{a}' = \mathbf{b}$ $\mathbf{b}' = \mathbf{c}_p$<br>Origin at $x, 0, 0$ | Along [010] $p2$<br>$\mathbf{a}' = \mathbf{c}$ $\mathbf{b}' = \mathbf{a}$<br>Origin at $0, y, 0$ |
|--|--|--|

**Maximal non-isomorphic subgroups**

**I** [2]  $P1(1)$  1

**IIa** none

**IIIb** none

**Maximal isomorphic subgroups of lowest index**

**IIIc** [2]  $P12_11$  ( $\mathbf{c}' = 2\mathbf{c}$  or  $\mathbf{a}' = 2\mathbf{a}$  or  $\mathbf{a}' = \mathbf{a} + \mathbf{c}, \mathbf{c}' = -\mathbf{a} + \mathbf{c}$ ) ( $P2_1, 4$ ); [3]  $P12_11$  ( $\mathbf{b}' = 3\mathbf{b}$ ) ( $P2_1, 4$ )

**Minimal non-isomorphic supergroups**

**I** [2]  $P2_1/m$  (11); [2]  $P2_1/c$  (14); [2]  $P222_1$  (17); [2]  $P2_12_12$  (18); [2]  $P2_12_12_1$  (19); [2]  $C222_1$  (20); [2]  $Pmc2_1$  (26); [2]  $Pca2_1$  (29); [2]  $Pmn2_1$  (31); [2]  $Pna2_1$  (33); [2]  $Cmc2_1$  (36); [2]  $P4_1$  (76); [2]  $P4_3$  (78); [3]  $P6_1$  (169); [3]  $P6_5$  (170); [3]  $P6_3$  (173)

**II** [2]  $C121$  ( $C2, 5$ ); [2]  $A121$  ( $C2, 5$ ); [2]  $I121$  ( $C2, 5$ ); [2]  $P121$  ( $\mathbf{b}' = \frac{1}{2}\mathbf{b}$ ) ( $P2, 3$ )

$P2_1$

No. 4

$C_2^2$

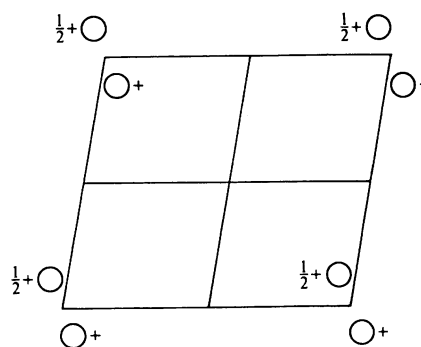
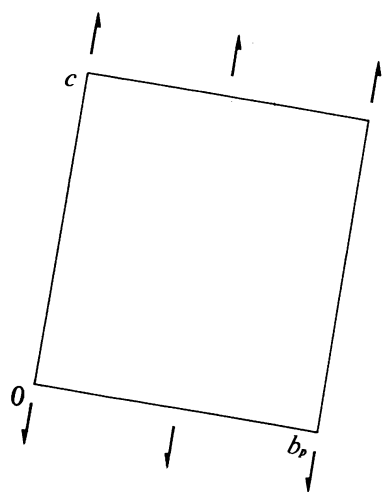
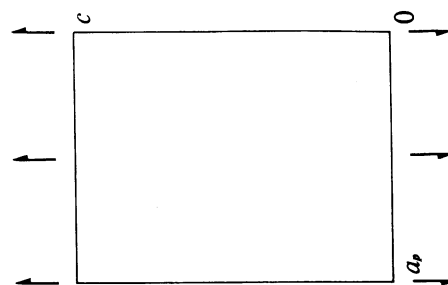
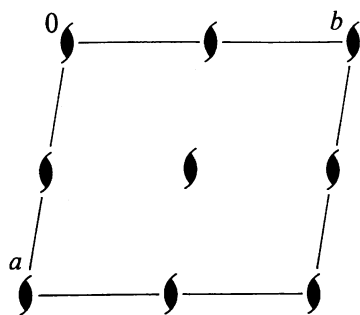
$P112_1$

2

Monoclinic

Patterson symmetry  $P112/m$

UNIQUE AXIS  $c$



Origin on  $2_1$

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

Symmetry operations

(1) 1 (2)  $2(0,0,\frac{1}{2}) 0,0,z$

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

**Positions**

| Multiplicity,<br>Wyckoff letter,<br>Site symmetry | Coordinates   | Reflection conditions |
|---|---|-----------------------|
|   |   | General:              |
| 2 $a$ 1   | (1) $x, y, z$ (2) $\bar{x}, \bar{y}, z + \frac{1}{2}$ | $00l : l = 2n$        |

**Symmetry of special projections**

|  |  |   |
|--|--|---|
| Along [001] $p2$<br>$\mathbf{a}' = \mathbf{a}$ $\mathbf{b}' = \mathbf{b}$<br>Origin at $0, 0, z$ | Along [100] $p1g1$<br>$\mathbf{a}' = \mathbf{b}_p$ $\mathbf{b}' = \mathbf{c}$<br>Origin at $x, 0, 0$ | Along [010] $p1g$<br>$\mathbf{a}' = \mathbf{c}$ $\mathbf{b}' = \mathbf{a}_p$<br>Origin at $0, y, 0$ |
|--|--|---|

**Maximal non-isomorphic subgroups**

- I** [2]  $P1(1)$  1  
**IIa** none  
**IIb** none

**Maximal isomorphic subgroups of lowest index**

- IIc** [2]  $P112_1$  ( $\mathbf{a}' = 2\mathbf{a}$  or  $\mathbf{b}' = 2\mathbf{b}$  or  $\mathbf{a}' = \mathbf{a} - \mathbf{b}, \mathbf{b}' = \mathbf{a} + \mathbf{b}$ ) ( $P2_1, 4$ ); [3]  $P112_1$  ( $\mathbf{c}' = 3\mathbf{c}$ ) ( $P2_1, 4$ )

**Minimal non-isomorphic supergroups**

- I** [2]  $P2_1/m$  (11); [2]  $P2_1/c$  (14); [2]  $P222_1$  (17); [2]  $P2_12_12$  (18); [2]  $P2_12_12_1$  (19); [2]  $C222_1$  (20); [2]  $Pmc2_1$  (26); [2]  $Pca2_1$  (29); [2]  $Pmn2_1$  (31); [2]  $Pna2_1$  (33); [2]  $Cmc2_1$  (36); [2]  $P4_1$  (76); [2]  $P4_3$  (78); [3]  $P6_1$  (169); [3]  $P6_5$  (170); [3]  $P6_3$  (173)  
**II** [2]  $A112$  ( $C2, 5$ ); [2]  $B112$  ( $C2, 5$ ); [2]  $I112$  ( $C2, 5$ ); [2]  $P112$  ( $\mathbf{c}' = \frac{1}{2}\mathbf{c}$ ) ( $P2, 3$ )