

$P2/c$

$C_{2h}^4$

$2/m$

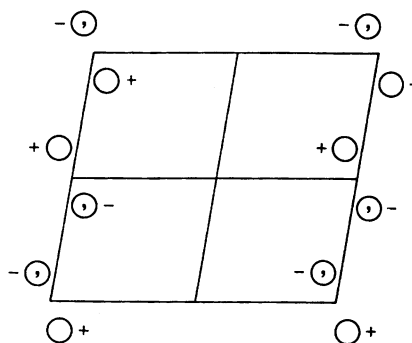
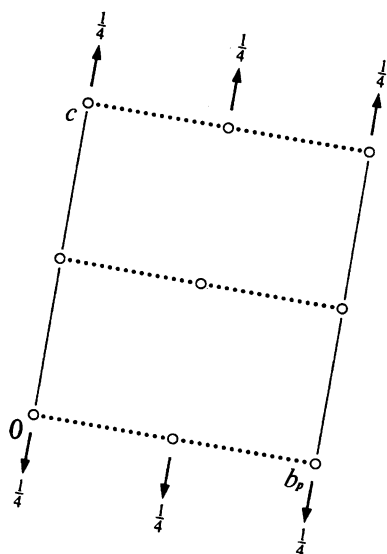
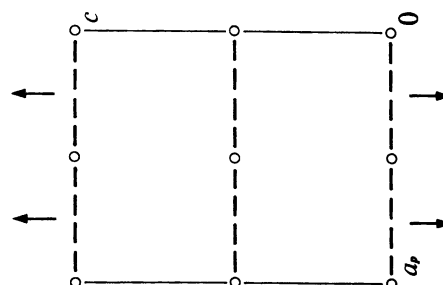
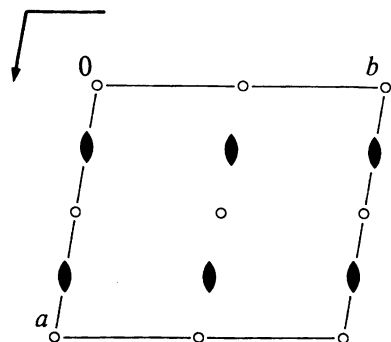
Monoclinic

No. 13

$P112/a$

Patterson symmetry  $P112/m$

UNIQUE AXIS  $c$ , CELL CHOICE 1



Origin at  $\bar{1}$  on glide plane  $a$

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

**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>g</i> 1	(1) $x,y,z$	(2) $\bar{x} + \frac{1}{2}, \bar{y}, z$	(3) $\bar{x}, \bar{y}, \bar{z}$	(4) $x + \frac{1}{2}, y, \bar{z}$	General: $hk0 : h = 2n$ $h00 : h = 2n$ Special: as above, plus no extra conditions
2 <i>f</i> 2	$\frac{1}{4}, \frac{1}{2}, z$	$\frac{3}{4}, \frac{1}{2}, \bar{z}$			no extra conditions
2 <i>e</i> 2	$\frac{1}{4}, 0, z$	$\frac{3}{4}, 0, \bar{z}$			no extra conditions
2 <i>d</i> $\bar{1}$	$0, \frac{1}{2}, 0$	$\frac{1}{2}, \frac{1}{2}, 0$			$hkl : h = 2n$
2 <i>c</i> $\bar{1}$	$0, 0, \frac{1}{2}$	$\frac{1}{2}, 0, \frac{1}{2}$			$hkl : h = 2n$
2 <i>b</i> $\bar{1}$	$0, \frac{1}{2}, \frac{1}{2}$	$\frac{1}{2}, \frac{1}{2}, \frac{1}{2}$			$hkl : h = 2n$
2 <i>a</i> $\bar{1}$	$0, 0, 0$	$\frac{1}{2}, 0, 0$			$hkl : h = 2n$

**Symmetry of special projections**

Along [001]  $p2$   
 $\mathbf{a}' = \frac{1}{2}\mathbf{a}$      $\mathbf{b}' = \mathbf{b}$   
Origin at 0,0,z

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

Along [010]  $p2gm$   
 $\mathbf{a}' = \mathbf{c}$      $\mathbf{b}' = \mathbf{a}_p$   
Origin at 0,y,0

**Maximal non-isomorphic subgroups**

**I** [2]  $P11a$  ( $Pc$ , 7) 1; 4  
[2]  $P112$  ( $P2$ , 3) 1; 2  
[2]  $P\bar{1}$  (2) 1; 3

**IIa** none

**IIb** [2]  $P112_1/a$  ( $\mathbf{c}' = 2\mathbf{c}$ ) ( $P2_1/c$ , 14); [2]  $A112/a$  ( $\mathbf{b}' = 2\mathbf{b}, \mathbf{c}' = 2\mathbf{c}$ ) ( $C2/c$ , 15)

**Maximal isomorphic subgroups of lowest index**

**IIc** [2]  $P112/a$  ( $\mathbf{c}' = 2\mathbf{c}$ ) ( $P2/c$ , 13); [2]  $P112/a$  ( $\mathbf{b}' = 2\mathbf{b}$  or  $\mathbf{a}' = \mathbf{a} + 2\mathbf{b}, \mathbf{b}' = 2\mathbf{b}$ ) ( $P2/c$ , 13)

**Minimal non-isomorphic supergroups**

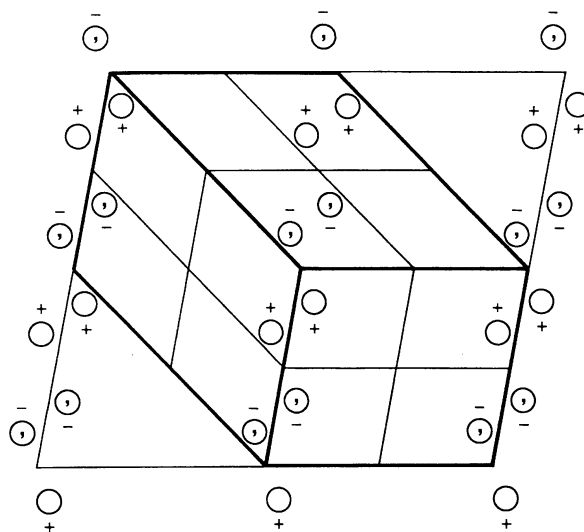
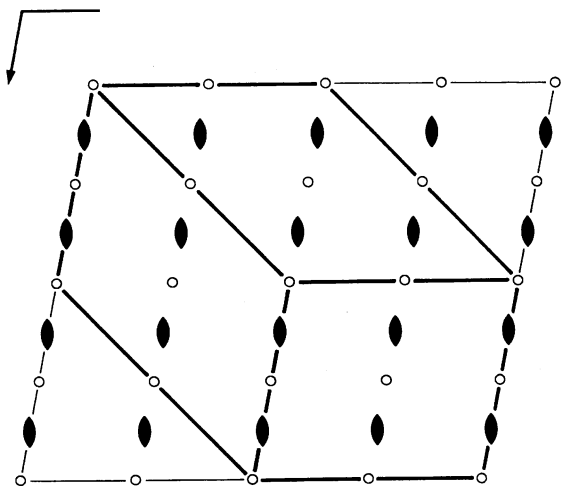
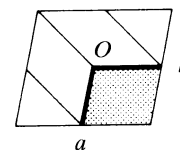
**I** [2]  $Pnnn$  (48); [2]  $Pccm$  (49); [2]  $Pban$  (50); [2]  $Pmma$  (51); [2]  $Pnna$  (52); [2]  $Pmna$  (53); [2]  $Pcca$  (54); [2]  $Pccn$  (56); [2]  $Pbcm$  (57); [2]  $Pmmn$  (59); [2]  $Pbcn$  (60); [2]  $Cmme$  (67); [2]  $Ccce$  (68); [2]  $P4/n$  (85); [2]  $P4_2/n$  (86)

**II** [2]  $A112/a$  ( $C2/c$ , 15); [2]  $B112/m$  ( $C2/m$ , 12); [2]  $I112/a$  ( $C2/c$ , 15); [2]  $P112/m$  ( $\mathbf{a}' = \frac{1}{2}\mathbf{a}$ ) ( $P2/m$ , 10)

$P2/c$  $C_{2h}^4$  $2/m$ 

Monoclinic

No. 13

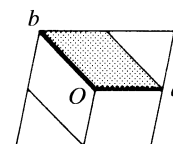
UNIQUE AXIS  $c$ , DIFFERENT CELL CHOICES $P112/a$ UNIQUE AXIS  $c$ , CELL CHOICE 1Origin at  $\bar{1}$  on glide plane  $a$ Asymmetric unit  $0 \leq x \leq \frac{1}{2}$ ;  $0 \leq y \leq \frac{1}{2}$ ;  $0 \leq z \leq 1$ Generators selected (1);  $t(1,0,0)$ ;  $t(0,1,0)$ ;  $t(0,0,1)$ ; (2); (3)**Positions**Multiplicity,  
Wyckoff letter,  
Site symmetry

Coordinates

Reflection conditions

Multiplicity, Wyckoff letter, Site symmetry	Coordinates	Reflection conditions
4 $g$ 1	(1) $x, y, z$ (2) $\bar{x} + \frac{1}{2}, \bar{y}, z$ (3) $\bar{x}, \bar{y}, \bar{z}$ (4) $x + \frac{1}{2}, y, \bar{z}$	General: $hk0 : h = 2n$ $h00 : h = 2n$
2 $f$ 2	$\frac{1}{4}, \frac{1}{2}, z$ $\frac{3}{4}, \frac{1}{2}, \bar{z}$	Special: as above, plus no extra conditions
2 $e$ 2	$\frac{1}{4}, 0, z$ $\frac{3}{4}, 0, \bar{z}$	no extra conditions
2 $d$ $\bar{1}$	$0, \frac{1}{2}, 0$ $\frac{1}{2}, \frac{1}{2}, 0$	$hkl : h = 2n$
2 $b$ $\bar{1}$	$0, \frac{1}{2}, \frac{1}{2}$ $\frac{1}{2}, \frac{1}{2}, \frac{1}{2}$	$hkl : h = 2n$
	2 $c$ $\bar{1}$ $0, 0, \frac{1}{2}$ $\frac{1}{2}, 0, \frac{1}{2}$	
	2 $a$ $\bar{1}$ $0, 0, 0$ $\frac{1}{2}, 0, 0$	

## P112/n

UNIQUE AXIS  $c$ , CELL CHOICE 2Origin at  $\bar{1}$  on glide plane  $n$ Asymmetric unit  $0 \leq x \leq \frac{1}{4}$ ;  $0 \leq y \leq 1$ ;  $0 \leq z \leq 1$ Generators selected (1);  $t(1,0,0)$ ;  $t(0,1,0)$ ;  $t(0,0,1)$ ; (2); (3)

## Positions

Multiplicity, Wyckoff letter, Site symmetry	Coordinates			
4 g 1	(1) $x, y, z$	(2) $\bar{x} + \frac{1}{2}, \bar{y} + \frac{1}{2}, z$	(3) $\bar{x}, \bar{y}, \bar{z}$	(4) $x + \frac{1}{2}, y + \frac{1}{2}, \bar{z}$
2 f 2	$\frac{1}{4}, \frac{3}{4}, z$	$\frac{3}{4}, \frac{1}{4}, \bar{z}$		
2 e 2	$\frac{3}{4}, \frac{3}{4}, z$	$\frac{1}{4}, \frac{1}{4}, \bar{z}$		
2 d $\bar{1}$	$\frac{1}{2}, 0, 0$	$0, \frac{1}{2}, 0$	2 c $\bar{1}$	$0, 0, \frac{1}{2}$ $\frac{1}{2}, \frac{1}{2}, \frac{1}{2}$
2 b $\bar{1}$	$\frac{1}{2}, 0, \frac{1}{2}$	$0, \frac{1}{2}, \frac{1}{2}$	2 a $\bar{1}$	$0, 0, 0$ $\frac{1}{2}, \frac{1}{2}, 0$

Reflection conditions

General:

$hk0 : h + k = 2n$

$h00 : h = 2n$

$0k0 : k = 2n$

Special: as above, plus

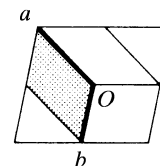
no extra conditions

no extra conditions

$hkl : h + k = 2n$

$hkl : h + k = 2n$

## P112/b

UNIQUE AXIS  $c$ , CELL CHOICE 3Origin at  $\bar{1}$  on glide plane  $b$ Asymmetric unit  $0 \leq x \leq \frac{1}{2}$ ;  $0 \leq y \leq \frac{1}{2}$ ;  $0 \leq z \leq 1$ Generators selected (1);  $t(1,0,0)$ ;  $t(0,1,0)$ ;  $t(0,0,1)$ ; (2); (3)

## Positions

Multiplicity, Wyckoff letter, Site symmetry	Coordinates			
4 g 1	(1) $x, y, z$	(2) $\bar{x}, \bar{y} + \frac{1}{2}, z$	(3) $\bar{x}, \bar{y}, \bar{z}$	(4) $x, y + \frac{1}{2}, \bar{z}$
2 f 2	$\frac{1}{2}, \frac{3}{4}, z$	$\frac{1}{2}, \frac{1}{4}, \bar{z}$		
2 e 2	$0, \frac{1}{4}, z$	$0, \frac{3}{4}, \bar{z}$		
2 d $\bar{1}$	$\frac{1}{2}, \frac{1}{2}, 0$	$\frac{1}{2}, 0, 0$	2 c $\bar{1}$	$0, 0, \frac{1}{2}$ $0, \frac{1}{2}, \frac{1}{2}$
2 b $\bar{1}$	$\frac{1}{2}, \frac{1}{2}, \frac{1}{2}$	$\frac{1}{2}, 0, \frac{1}{2}$	2 a $\bar{1}$	$0, 0, 0$ $0, \frac{1}{2}, 0$

Reflection conditions

General:

$hk0 : k = 2n$

$0k0 : k = 2n$

Special: as above, plus

no extra conditions

no extra conditions

$hkl : k = 2n$

$hkl : k = 2n$