

$P2/c$

$C_{2h}^4$

$2/m$

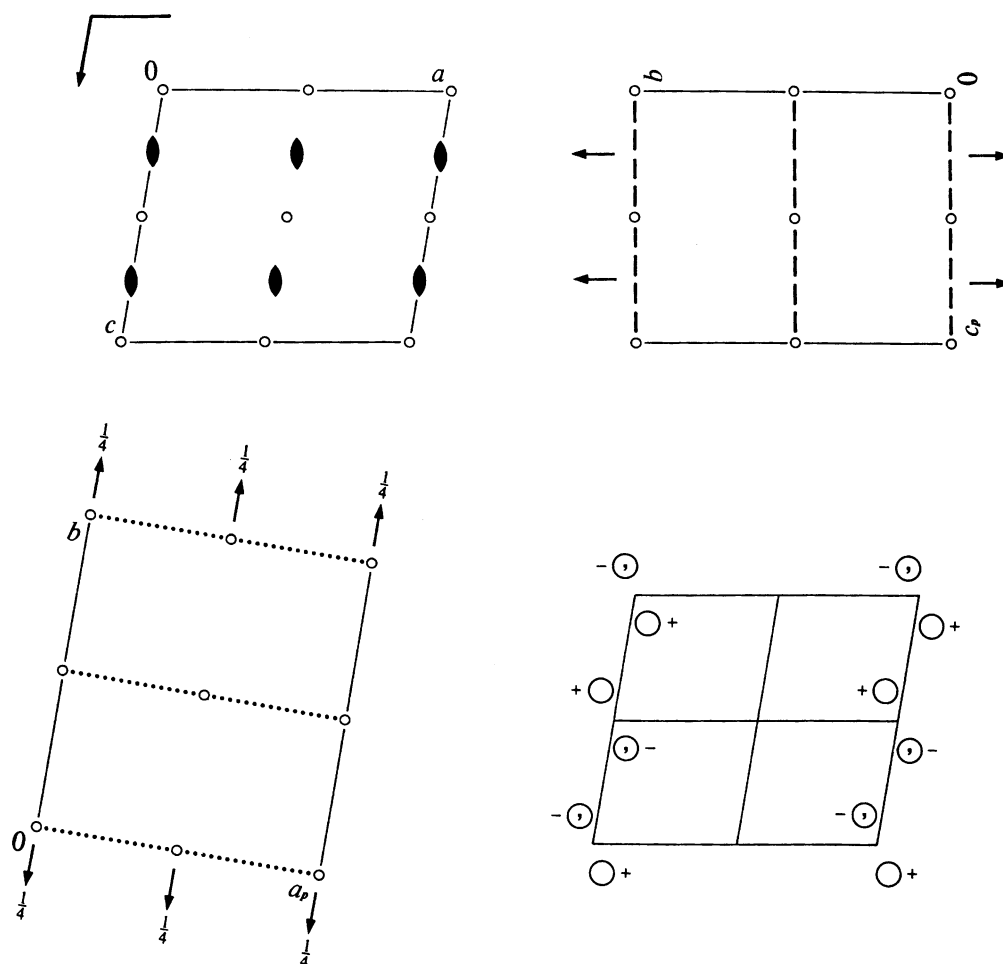
Monoclinic

No. 13

$P12/c1$

Patterson symmetry  $P12/m1$

UNIQUE AXIS  $b$ , CELL CHOICE 1



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

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

Symmetry operations

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

**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) $\bar{x}, y, \bar{z} + \frac{1}{2}$	(3) $\bar{x}, \bar{y}, \bar{z}$	(4) $x, \bar{y}, z + \frac{1}{2}$
2	<i>f</i>	2	$\frac{1}{2}, y, \frac{1}{4}$	$\frac{1}{2}, \bar{y}, \frac{3}{4}$		
2	<i>e</i>	2	$0, y, \frac{1}{4}$	$0, \bar{y}, \frac{3}{4}$		
2	<i>d</i>	$\bar{1}$	$\frac{1}{2}, 0, 0$	$\frac{1}{2}, 0, \frac{1}{2}$		
2	<i>c</i>	$\bar{1}$	$0, \frac{1}{2}, 0$	$0, \frac{1}{2}, \frac{1}{2}$		
2	<i>b</i>	$\bar{1}$	$\frac{1}{2}, \frac{1}{2}, 0$	$\frac{1}{2}, \frac{1}{2}, \frac{1}{2}$		
2	<i>a</i>	$\bar{1}$	$0, 0, 0$	$0, 0, \frac{1}{2}$		

General:

$$h0l: l = 2n$$

$$00l: l = 2n$$

Special: as above, plus

no extra conditions

no extra conditions

$$hkl: l = 2n$$

$$hkl: l = 2n$$

$$hkl: l = 2n$$

$$hkl: l = 2n$$

**Symmetry of special projections**

Along [001]  $p2mm$

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

Origin at  $0, 0, z$

Along [100]  $p2gm$

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

Origin at  $x, 0, 0$

Along [010]  $p2$

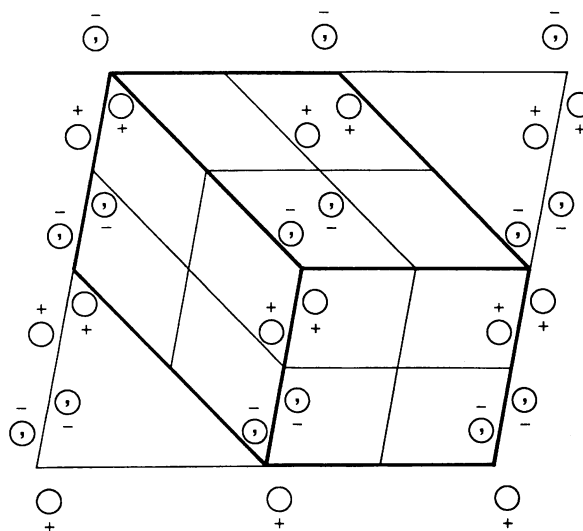
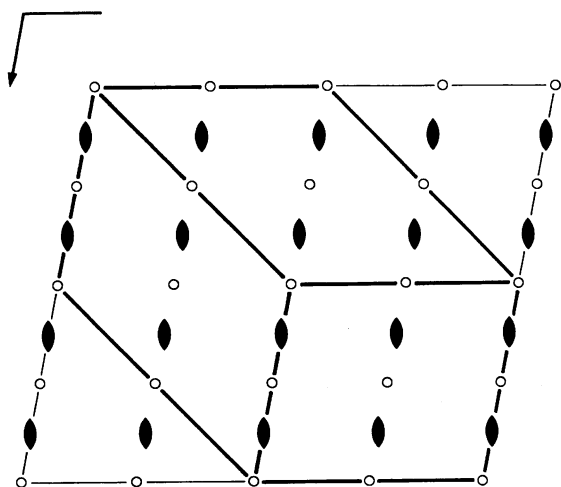
$$\mathbf{a}' = \frac{1}{2}\mathbf{c} \quad \mathbf{b}' = \mathbf{a}$$

Origin at  $0, y, 0$

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

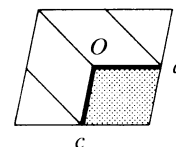
Monoclinic

No. 13

UNIQUE AXIS  $b$ , DIFFERENT CELL CHOICES $P12/c1$ UNIQUE AXIS  $b$ , CELL CHOICE 1Origin at  $\bar{1}$  on glide plane  $c$ Asymmetric unit  $0 \leq x \leq \frac{1}{2}$ ;  $0 \leq y \leq 1$ ;  $0 \leq z \leq \frac{1}{2}$ Generators selected (1);  $t(1,0,0)$ ;  $t(0,1,0)$ ;  $t(0,0,1)$ ; (2); (3)**Positions**Multiplicity,  
Wyckoff letter,  
Site symmetry

Coordinates

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



Reflection conditions

General:

 $h0l: l = 2n$  $00l: l = 2n$ 

Special: as above, plus

no extra conditions

no extra conditions

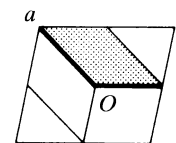
 $hkl: l = 2n$  $hkl: l = 2n$

## P12/n1

UNIQUE AXIS  $b$ , CELL CHOICE 2**Origin** at  $\bar{1}$  on glide plane  $n$ **Asymmetric unit**  $0 \leq x \leq 1; 0 \leq y \leq 1; 0 \leq z \leq \frac{1}{4}$ **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) $\bar{x} + \frac{1}{2}, y, \bar{z} + \frac{1}{2}$	(3) $\bar{x}, \bar{y}, \bar{z}$	(4) $x + \frac{1}{2}, \bar{y}, z + \frac{1}{2}$
2	$f$	2	$\frac{3}{4}, y, \frac{1}{4}$	$\frac{1}{4}, \bar{y}, \frac{3}{4}$		
2	$e$	2	$\frac{3}{4}, y, \frac{3}{4}$	$\frac{1}{4}, \bar{y}, \frac{1}{4}$		
2	$d$	$\bar{1}$	$0, 0, \frac{1}{2}$	$\frac{1}{2}, 0, 0$	2	$c$ $\bar{1}$ $0, \frac{1}{2}, 0$ $\frac{1}{2}, \frac{1}{2}, \frac{1}{2}$
2	$b$	$\bar{1}$	$0, \frac{1}{2}, \frac{1}{2}$	$\frac{1}{2}, \frac{1}{2}, 0$	2	$a$ $\bar{1}$ $0, 0, 0$ $\frac{1}{2}, 0, \frac{1}{2}$



Reflection conditions

General:

$$h0l: h + l = 2n$$

$$h00: h = 2n$$

$$00l: l = 2n$$

Special: as above, plus

no extra conditions

no extra conditions

$$hkl: h + l = 2n$$

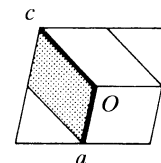
$$hkl: h + l = 2n$$

## P12/a1

UNIQUE AXIS  $b$ , CELL CHOICE 3**Origin** at  $\bar{1}$  on glide plane  $a$ **Asymmetric unit**  $0 \leq x \leq \frac{1}{2}; 0 \leq y \leq 1; 0 \leq z \leq \frac{1}{2}$ **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) $\bar{x} + \frac{1}{2}, y, \bar{z}$	(3) $\bar{x}, \bar{y}, \bar{z}$	(4) $x + \frac{1}{2}, \bar{y}, z$
2	$f$	2	$\frac{3}{4}, y, \frac{1}{2}$	$\frac{1}{4}, \bar{y}, \frac{1}{2}$		
2	$e$	2	$\frac{1}{4}, y, 0$	$\frac{3}{4}, \bar{y}, 0$		
2	$d$	$\bar{1}$	$\frac{1}{2}, 0, \frac{1}{2}$	$0, 0, \frac{1}{2}$	2	$c$ $\bar{1}$ $0, \frac{1}{2}, 0$ $\frac{1}{2}, \frac{1}{2}, 0$
2	$b$	$\bar{1}$	$\frac{1}{2}, \frac{1}{2}, \frac{1}{2}$	$0, \frac{1}{2}, \frac{1}{2}$	2	$a$ $\bar{1}$ $0, 0, 0$ $\frac{1}{2}, 0, 0$



Reflection conditions

General:

$$h0l: h = 2n$$

$$h00: h = 2n$$

Special: as above, plus

no extra conditions

no extra conditions

$$hkl: h = 2n$$

$$hkl: h = 2n$$

$P2/c$

$C_{2h}^4$

$2/m$

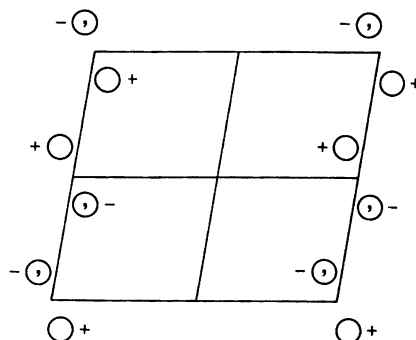
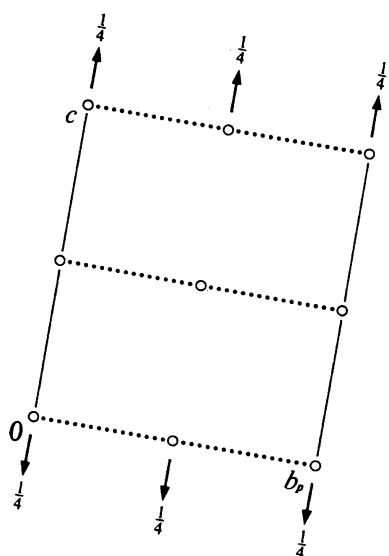
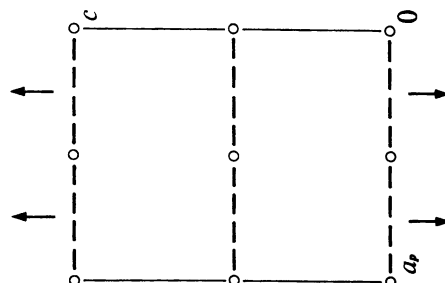
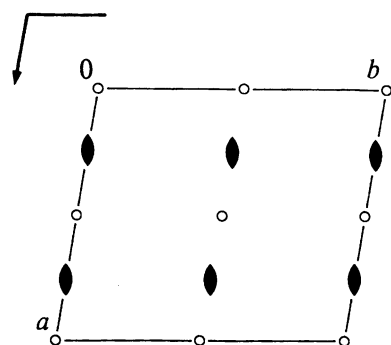
Monoclinic

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 no extra conditions $hkl: h = 2n$ $hkl: h = 2n$ $hkl: h = 2n$ $hkl: h = 2n$
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  $0, 0, z$

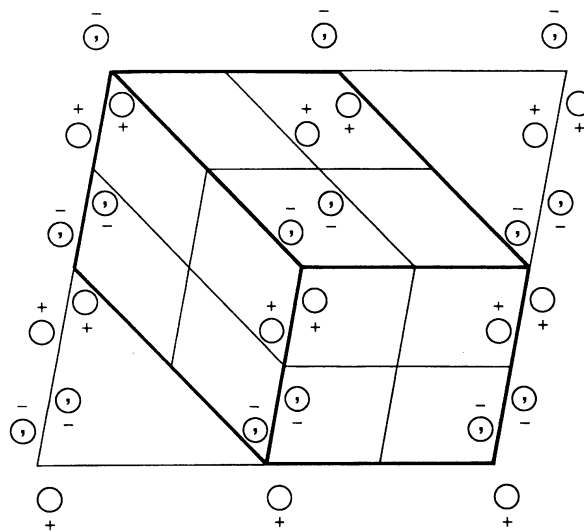
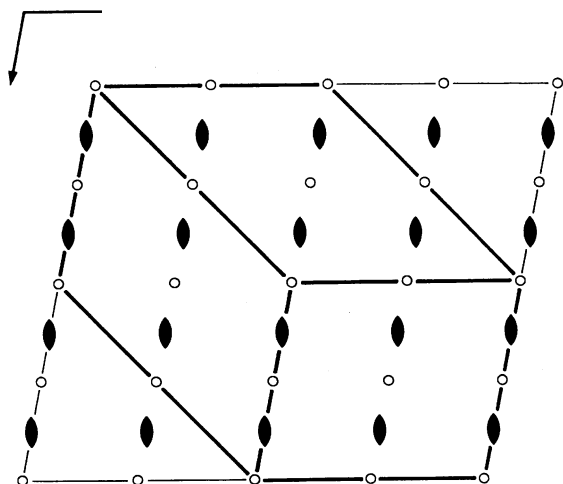
Along [100]  $p2mm$   
 $\mathbf{a}' = \mathbf{b}'_p$      $\mathbf{b}' = \mathbf{c}$   
 Origin at  $x, 0, 0$

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

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

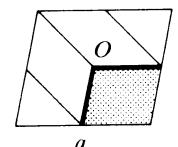
Monoclinic

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

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



Reflection conditions

General:

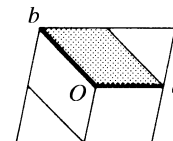
 $hk0: h = 2n$  $h00: h = 2n$ 

Special: as above, plus

no extra conditions

no extra conditions

 $hkl: h = 2n$  $hkl: h = 2n$

**P112/n**UNIQUE AXIS  $c$ , CELL CHOICE 2**Origin** 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:

$hk0: h + k = 2n$

$h00: h = 2n$

$0k0: k = 2n$

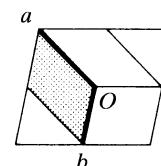
Special: as above, plus

no extra conditions

no extra conditions

$hkl: h + k = 2n$

$hkl: h + k = 2n$

**P112/b**UNIQUE AXIS  $c$ , CELL CHOICE 3**Origin** 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

$hkl: k = 2n$

$hkl: k = 2n$