

$C2/m$

C_{2h}^3

$2/m$

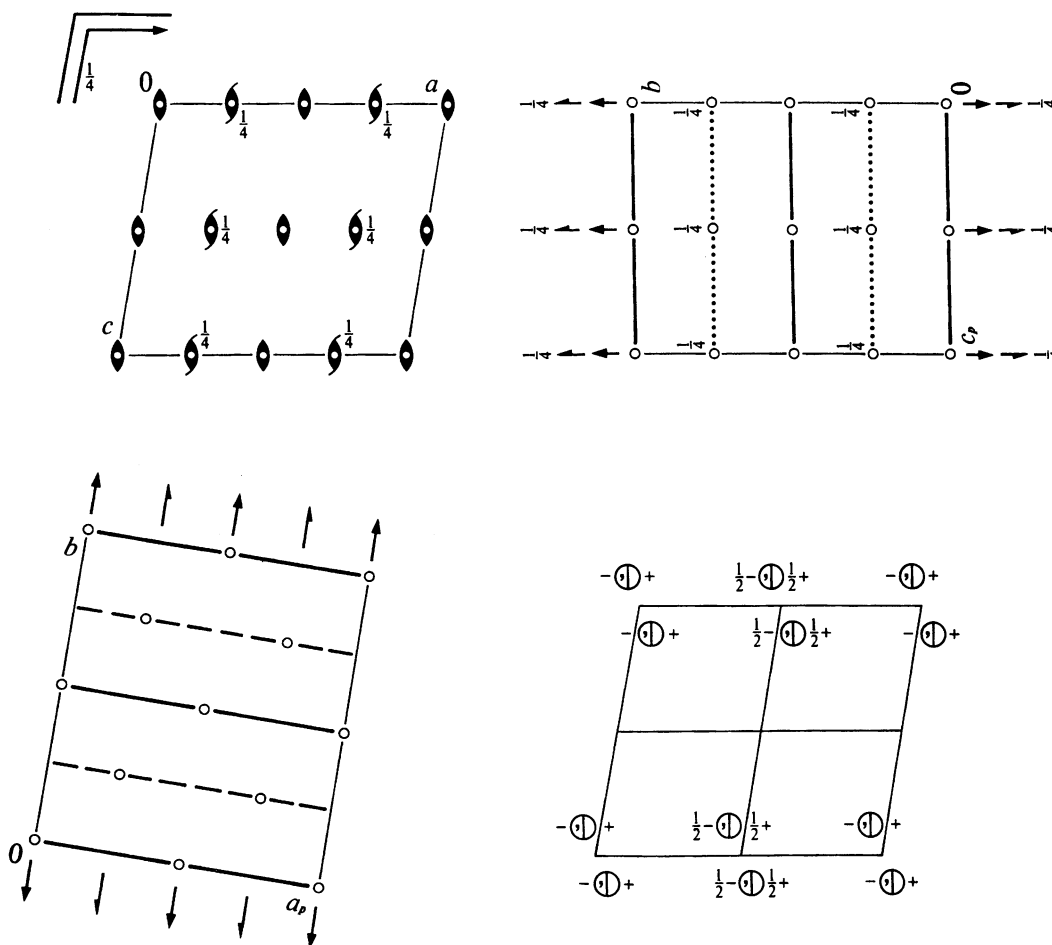
Monoclinic

No. 12

$C12/m1$

Patterson symmetry $C12/m1$

UNIQUE AXIS b , CELL CHOICE 1



Origin at centre ($2/m$)

Asymmetric unit $0 \leq x \leq \frac{1}{2}; 0 \leq y \leq \frac{1}{4}; 0 \leq z \leq 1$

Symmetry operations

For $(0,0,0)+$ set

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

For $(\frac{1}{2},\frac{1}{2},0)+$ set

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

Generators selected (1); $t(1,0,0)$; $t(0,1,0)$; $t(0,0,1)$; $t(\frac{1}{2}, \frac{1}{2}, 0)$; (2); (3)

Positions

Multiplicity, Wyckoff letter, Site symmetry		Coordinates				Reflection conditions
		$(0,0,0) + (\frac{1}{2}, \frac{1}{2}, 0) +$				General:
8	j 1	(1) x, y, z	(2) \bar{x}, y, \bar{z}	(3) $\bar{x}, \bar{y}, \bar{z}$	(4) x, \bar{y}, z	$hkl: h + k = 2n$ $h0l: h = 2n$ $0kl: k = 2n$ $hk0: h + k = 2n$ $0k0: k = 2n$ $h00: h = 2n$ Special: as above, plus no extra conditions
4	i m	$x, 0, z$	$\bar{x}, 0, \bar{z}$			no extra conditions
4	h 2	$0, y, \frac{1}{2}$	$0, \bar{y}, \frac{1}{2}$			no extra conditions
4	g 2	$0, y, 0$	$0, \bar{y}, 0$			no extra conditions
4	f $\bar{1}$	$\frac{1}{4}, \frac{1}{4}, \frac{1}{2}$	$\frac{3}{4}, \frac{1}{4}, \frac{1}{2}$			$hkl: h = 2n$
4	e $\bar{1}$	$\frac{1}{4}, \frac{1}{4}, 0$	$\frac{3}{4}, \frac{1}{4}, 0$			$hkl: h = 2n$
2	d $2/m$	$0, \frac{1}{2}, \frac{1}{2}$				no extra conditions
2	c $2/m$	$0, 0, \frac{1}{2}$				no extra conditions
2	b $2/m$	$0, \frac{1}{2}, 0$				no extra conditions
2	a $2/m$	$0, 0, 0$				no extra conditions

Symmetry of special projections

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

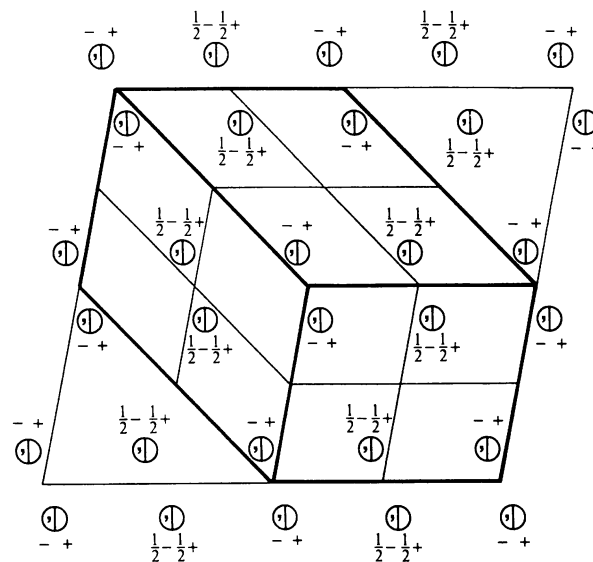
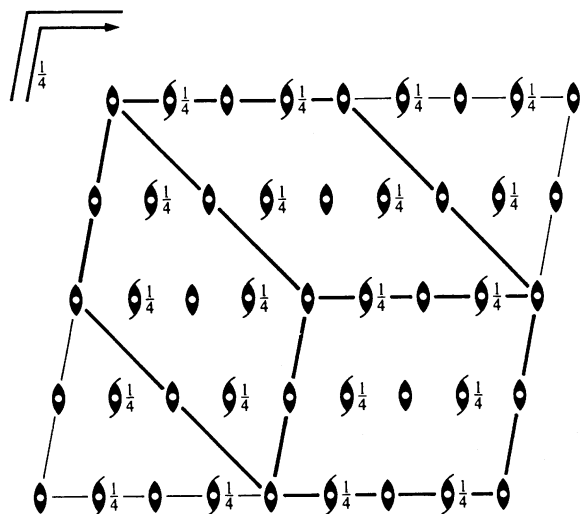
Along $[100]$ $p2mm$
 $\mathbf{a}' = \frac{1}{2}\mathbf{b}$ $\mathbf{b}' = \mathbf{c}_p$
 Origin at $x, 0, 0$

Along $[010]$ $p2$
 $\mathbf{a}' = \mathbf{c}$ $\mathbf{b}' = \frac{1}{2}\mathbf{a}$
 Origin at $0, y, 0$

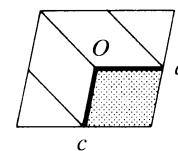
$C2/m$ C_{2h}^3 $2/m$

Monoclinic

No. 12

UNIQUE AXIS b , DIFFERENT CELL CHOICES $C12/m1$ UNIQUE AXIS b , CELL CHOICE 1Origin at centre ($2/m$)Asymmetric unit $0 \leq x \leq \frac{1}{2}$; $0 \leq y \leq \frac{1}{4}$; $0 \leq z \leq 1$ Generators selected (1); $t(1,0,0)$; $t(0,1,0)$; $t(0,0,1)$; $t(\frac{1}{2}, \frac{1}{2}, 0)$; (2); (3)**Positions**Multiplicity,
Wyckoff letter,
Site symmetry

Coordinates

 $(0,0,0)+$ $(\frac{1}{2}, \frac{1}{2}, 0)+$ 8 j 1 (1) x, y, z (2) \bar{x}, y, \bar{z} (3) $\bar{x}, \bar{y}, \bar{z}$ (4) x, \bar{y}, z 4 i m $x, 0, z$ $\bar{x}, 0, \bar{z}$ 4 h 2 $0, y, \frac{1}{2}$ $0, \bar{y}, \frac{1}{2}$ 4 g 2 $0, y, 0$ $0, \bar{y}, 0$ 4 f $\bar{1}$ $\frac{1}{4}, \frac{1}{4}, \frac{1}{2}$ $\frac{3}{4}, \frac{1}{4}, \frac{1}{2}$ 4 e $\bar{1}$ $\frac{1}{4}, \frac{1}{4}, 0$ $\frac{3}{4}, \frac{1}{4}, 0$ 2 d $2/m$ $0, \frac{1}{2}, \frac{1}{2}$ 2 c $2/m$ $0, 0, \frac{1}{2}$ 2 b $2/m$ $0, \frac{1}{2}, 0$ 2 a $2/m$ $0, 0, 0$ 

Reflection conditions

General:

 hkl : $h+k=2n$ $hk0$: $h+k=2n$ $h0l$: $h=2n$ $0k0$: $k=2n$ $0kl$: $k=2n$ $h00$: $h=2n$

Special: as above, plus

no extra conditions

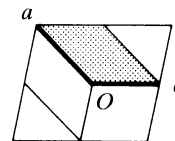
no extra conditions

 hkl : $h=2n$

no extra conditions

no extra conditions

A 12/m 1

UNIQUE AXIS b , CELL CHOICE 2Origin at centre ($2/m$)Asymmetric unit $0 \leq x \leq \frac{1}{2}$; $0 \leq y \leq \frac{1}{4}$; $0 \leq z \leq 1$ Generators selected (1); $t(1,0,0)$; $t(0,1,0)$; $t(0,0,1)$; $t(0, \frac{1}{2}, \frac{1}{2})$; (2); (3)

Positions

Multiplicity,
Wyckoff letter,
Site symmetry

Coordinates

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

Reflection conditions

General:

8 j 1 (1) x, y, z (2) \bar{x}, y, \bar{z} (3) $\bar{x}, \bar{y}, \bar{z}$ (4) x, \bar{y}, z
 $hkl: k+l=2n$ $hk0: k=2n$
 $h0l: l=2n$ $0k0: k=2n$
 $0kl: k+l=2n$ $00l: l=2n$

Special: as above, plus

4	i	m	$x, 0, z$	$\bar{x}, 0, \bar{z}$				
4	h	2	$\frac{1}{2}, y, \frac{1}{2}$	$\frac{1}{2}, \bar{y}, \frac{1}{2}$	4	g	2	$0, y, 0$ $0, \bar{y}, 0$
4	f	$\bar{1}$	$\frac{1}{2}, \frac{1}{4}, \frac{3}{4}$	$\frac{1}{2}, \frac{1}{4}, \frac{1}{4}$	4	e	$\bar{1}$	$0, \frac{1}{4}, \frac{1}{4}$ $0, \frac{1}{4}, \frac{3}{4}$
2	d	$2/m$	$\frac{1}{2}, \frac{1}{2}, \frac{1}{2}$		2	c	$2/m$	$\frac{1}{2}, 0, \frac{1}{2}$
2	b	$2/m$	$0, \frac{1}{2}, 0$		2	a	$2/m$	$0, 0, 0$

no extra conditions

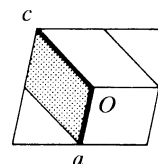
no extra conditions

 $hkl: k=2n$

no extra conditions

no extra conditions

I 12/m 1

UNIQUE AXIS b , CELL CHOICE 3Origin at centre ($2/m$)Asymmetric unit $0 \leq x \leq \frac{1}{2}$; $0 \leq y \leq \frac{1}{4}$; $0 \leq z \leq 1$ Generators selected (1); $t(1,0,0)$; $t(0,1,0)$; $t(0,0,1)$; $t(\frac{1}{2}, \frac{1}{2}, \frac{1}{2})$; (2); (3)

Positions

Multiplicity,
Wyckoff letter,
Site symmetry

Coordinates

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

Reflection conditions

General:

8 j 1 (1) x, y, z (2) \bar{x}, y, \bar{z} (3) $\bar{x}, \bar{y}, \bar{z}$ (4) x, \bar{y}, z
 $hkl: h+k+l=2n$ $0k0: k=2n$
 $h0l: h+l=2n$ $h00: h=2n$
 $0kl: k+l=2n$ $00l: l=2n$
 $hk0: h+k=2n$

Special: as above, plus

4	i	m	$x, 0, z$	$\bar{x}, 0, \bar{z}$				
4	h	2	$\frac{1}{2}, y, 0$	$\frac{1}{2}, \bar{y}, 0$	4	g	2	$0, y, 0$ $0, \bar{y}, 0$
4	f	$\bar{1}$	$\frac{1}{4}, \frac{1}{4}, \frac{3}{4}$	$\frac{3}{4}, \frac{1}{4}, \frac{1}{4}$	4	e	$\bar{1}$	$\frac{3}{4}, \frac{1}{4}, \frac{3}{4}$ $\frac{1}{4}, \frac{1}{4}, \frac{1}{4}$
2	d	$2/m$	$\frac{1}{2}, \frac{1}{2}, 0$		2	c	$2/m$	$\frac{1}{2}, 0, 0$
2	b	$2/m$	$0, \frac{1}{2}, 0$		2	a	$2/m$	$0, 0, 0$

no extra conditions

no extra conditions

 $hkl: k=2n$

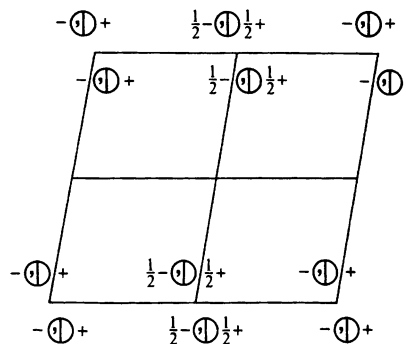
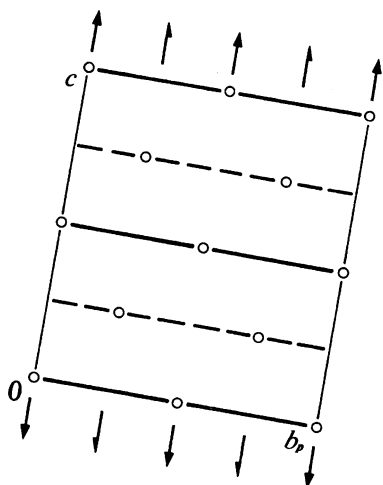
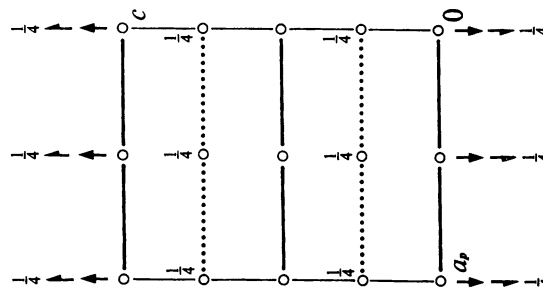
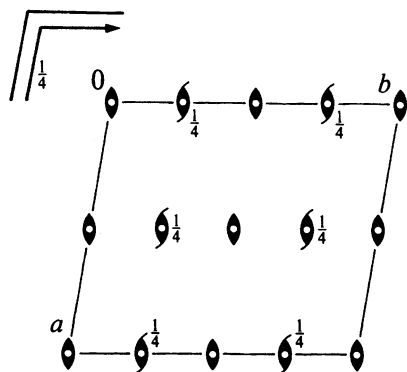
no extra conditions

no extra conditions

$C2/m$ C_{2h}^3 $2/m$

Monoclinic

No. 12

 $A112/m$ Patterson symmetry $A112/m$ UNIQUE AXIS c , CELL CHOICE 1**Origin** at centre ($2/m$)**Asymmetric unit** $0 \leq x \leq 1; 0 \leq y \leq \frac{1}{2}; 0 \leq z \leq \frac{1}{4}$ **Symmetry operations**For $(0,0,0)+$ set

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

For $(0, \frac{1}{2}, \frac{1}{2})+$ set

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

Generators selected (1); $t(1,0,0)$; $t(0,1,0)$; $t(0,0,1)$; $t(0, \frac{1}{2}, \frac{1}{2})$; (2); (3)

Positions

Multiplicity, Wyckoff letter, Site symmetry		Coordinates				Reflection conditions
		$(0,0,0) + (0, \frac{1}{2}, \frac{1}{2}) +$				General:
8	<i>j</i> 1	(1) x, y, z	(2) \bar{x}, \bar{y}, z	(3) $\bar{x}, \bar{y}, \bar{z}$	(4) x, y, \bar{z}	$hkl: k + l = 2n$ $hk0: k = 2n$ $0kl: k + l = 2n$ $h0l: l = 2n$ $00l: l = 2n$ $0k0: k = 2n$
4	<i>i</i> <i>m</i>	$x, y, 0$	$\bar{x}, \bar{y}, 0$			Special: as above, plus no extra conditions
4	<i>h</i> 2	$\frac{1}{2}, 0, z$	$\frac{1}{2}, 0, \bar{z}$			no extra conditions
4	<i>g</i> 2	$0, 0, z$	$0, 0, \bar{z}$			no extra conditions
4	<i>f</i> $\bar{1}$	$\frac{1}{2}, \frac{1}{4}, \frac{1}{4}$	$\frac{1}{2}, \frac{3}{4}, \frac{1}{4}$			$hkl: k = 2n$
4	<i>e</i> $\bar{1}$	$0, \frac{1}{4}, \frac{1}{4}$	$0, \frac{3}{4}, \frac{1}{4}$			$hkl: k = 2n$
2	<i>d</i> $2/m$	$\frac{1}{2}, 0, \frac{1}{2}$				no extra conditions
2	<i>c</i> $2/m$	$\frac{1}{2}, 0, 0$				no extra conditions
2	<i>b</i> $2/m$	$0, 0, \frac{1}{2}$				no extra conditions
2	<i>a</i> $2/m$	$0, 0, 0$				no extra conditions

Symmetry of special projections

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

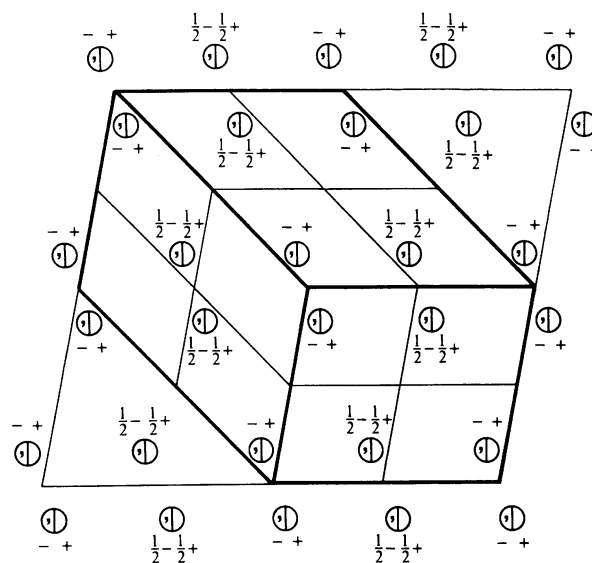
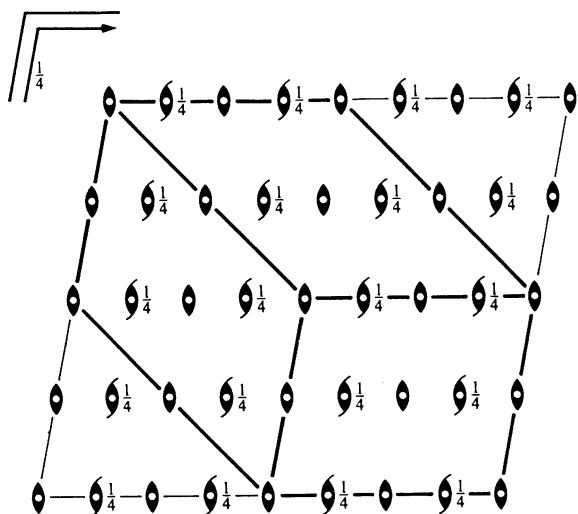
Along $[100]$ $c2mm$
 $\mathbf{a}' = \mathbf{b}_p$ $\mathbf{b}' = \mathbf{c}$
 Origin at $x, 0, 0$

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

$C2/m$ C_{2h}^3 $2/m$

Monoclinic

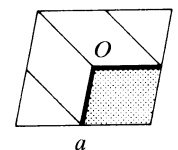
No. 12

UNIQUE AXIS c , DIFFERENT CELL CHOICES $A112/m$ UNIQUE AXIS c , CELL CHOICE 1Origin at centre ($2/m$)Asymmetric unit $0 \leq x \leq 1$; $0 \leq y \leq \frac{1}{2}$; $0 \leq z \leq \frac{1}{4}$ Generators selected (1); $t(1,0,0)$; $t(0,1,0)$; $t(0,0,1)$; $t(0, \frac{1}{2}, \frac{1}{2})$; (2); (3)

Positions

Multiplicity,
Wyckoff letter,
Site symmetry

Coordinates

 $(0,0,0)+$ $(0, \frac{1}{2}, \frac{1}{2})+$ 8 j 1 (1) x, y, z (2) \bar{x}, \bar{y}, z (3) $\bar{x}, \bar{y}, \bar{z}$ (4) x, y, \bar{z} 4 i m $x, y, 0$ $\bar{x}, \bar{y}, 0$ 4 h 2 $\frac{1}{2}, 0, z$ $\frac{1}{2}, 0, \bar{z}$ 4 g 2 $0, 0, z$ $0, 0, \bar{z}$ 4 f $\bar{1}$ $\frac{1}{2}, \frac{1}{4}, \frac{1}{4}$ $\frac{1}{2}, \frac{3}{4}, \frac{1}{4}$ 4 e $\bar{1}$ $0, \frac{1}{4}, \frac{1}{4}$ $0, \frac{3}{4}, \frac{1}{4}$ 2 d $2/m$ $\frac{1}{2}, 0, \frac{1}{2}$ 2 c $2/m$ $\frac{1}{2}, 0, 0$ no extra conditions2 b $2/m$ $0, 0, \frac{1}{2}$ 2 a $2/m$ $0, 0, 0$ no extra conditions

Reflection conditions

General:

 hkl : $k+l=2n$ $h0l$: $l=2n$ $hk0$: $k=2n$ $00l$: $l=2n$ $0kl$: $k+l=2n$ $0k0$: $k=2n$

Special: as above, plus

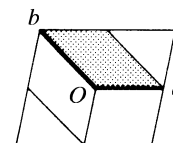
no extra conditions

no extra conditions

 hkl : $k=2n$

no extra conditions

no extra conditions

B112/mUNIQUE AXIS c , CELL CHOICE 2**Origin** at centre ($2/m$)**Asymmetric unit** $0 \leq x \leq 1$; $0 \leq y \leq \frac{1}{2}$; $0 \leq z \leq \frac{1}{4}$ **Generators selected** (1) ; $t(1,0,0)$; $t(0,1,0)$; $t(0,0,1)$; $t(\frac{1}{2},0,\frac{1}{2})$; (2) ; (3) **Positions**Multiplicity,
Wyckoff letter,
Site symmetry

Coordinates

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

Reflection conditions

General:

8 j 1 (1) x,y,z (2) \bar{x},\bar{y},z (3) \bar{x},\bar{y},\bar{z} (4) x,y,\bar{z}
 $hkl: h+l=2n$ $h0l: h+l=2n$
 $hk0: h=2n$ $00l: l=2n$
 $0kl: l=2n$ $h00: h=2n$

Special: as above, plus

4 i m $x,y,0$ $\bar{x},\bar{y},0$

no extra conditions

4 h 2 $\frac{1}{2},\frac{1}{2},z$ $\frac{1}{2},\frac{1}{2},\bar{z}$ 4 g 2 $0,0,z$ $0,0,\bar{z}$

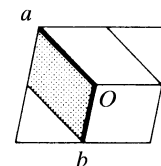
no extra conditions

4 f $\bar{1}$ $\frac{3}{4},\frac{1}{2},\frac{1}{4}$ $\frac{1}{4},\frac{1}{2},\frac{1}{4}$ 4 e $\bar{1}$ $\frac{1}{4},0,\frac{1}{4}$ $\frac{3}{4},0,\frac{1}{4}$ $hkl: h=2n$ 2 d $2/m$ $\frac{1}{2},\frac{1}{2},\frac{1}{2}$ 2 c $2/m$ $\frac{1}{2},\frac{1}{2},0$

no extra conditions

2 b $2/m$ $0,0,\frac{1}{2}$ 2 a $2/m$ $0,0,0$

no extra conditions

I112/mUNIQUE AXIS c , CELL CHOICE 3**Origin** at centre ($2/m$)**Asymmetric unit** $0 \leq x \leq 1$; $0 \leq y \leq \frac{1}{2}$; $0 \leq z \leq \frac{1}{4}$ **Generators selected** (1) ; $t(1,0,0)$; $t(0,1,0)$; $t(0,0,1)$; $t(\frac{1}{2},\frac{1}{2},\frac{1}{2})$; (2) ; (3) **Positions**Multiplicity,
Wyckoff letter,
Site symmetry

Coordinates

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

Reflection conditions

General:

8 j 1 (1) x,y,z (2) \bar{x},\bar{y},z (3) \bar{x},\bar{y},\bar{z} (4) x,y,\bar{z}
 $hkl: h+k+l=2n$ $00l: l=2n$
 $hk0: h+k=2n$ $h00: h=2n$
 $0kl: k+l=2n$ $0k0: k=2n$
 $h0l: h+l=2n$

Special: as above, plus

4 i m $x,y,0$ $\bar{x},\bar{y},0$

no extra conditions

4 h 2 $0,\frac{1}{2},z$ $0,\frac{1}{2},\bar{z}$ 4 g 2 $0,0,z$ $0,0,\bar{z}$

no extra conditions

4 f $\bar{1}$ $\frac{3}{4},\frac{1}{4},\frac{1}{4}$ $\frac{1}{4},\frac{3}{4},\frac{1}{4}$ 4 e $\bar{1}$ $\frac{3}{4},\frac{3}{4},\frac{1}{4}$ $\frac{1}{4},\frac{1}{4},\frac{1}{4}$ $hkl: l=2n$ 2 d $2/m$ $0,\frac{1}{2},\frac{1}{2}$ 2 c $2/m$ $0,\frac{1}{2},0$

no extra conditions

2 b $2/m$ $0,0,\frac{1}{2}$ 2 a $2/m$ $0,0,0$

no extra conditions