

$P2/c$

C_{2h}^4

$2/m$

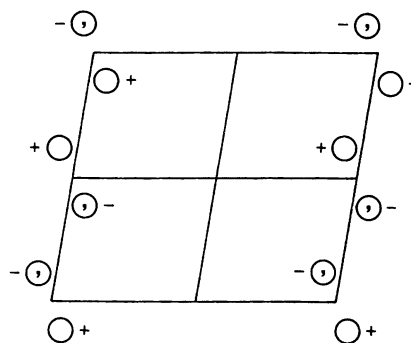
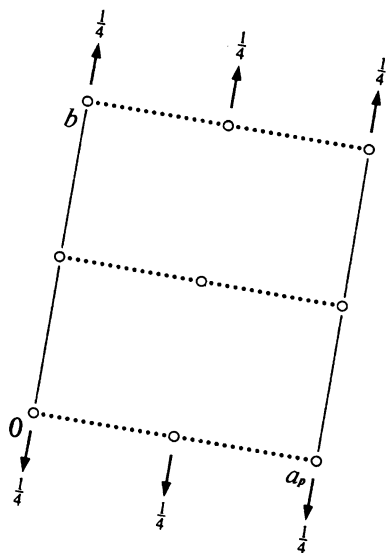
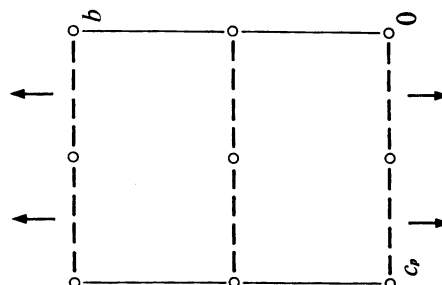
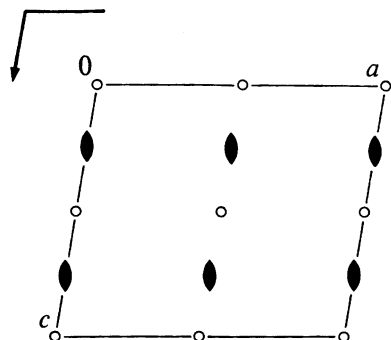
Monoclinic

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) $x, \bar{y}, z + \frac{1}{2}$	General: $h0l : l = 2n$ $00l : l = 2n$ Special: as above, plus no extra conditions
2	<i>f</i> 2	$\frac{1}{2}, y, \frac{1}{4}$	$\frac{1}{2}, \bar{y}, \frac{3}{4}$			no extra conditions
2	<i>e</i> 2	$0, y, \frac{1}{4}$	$0, \bar{y}, \frac{3}{4}$			no extra conditions
2	<i>d</i> $\bar{1}$	$\frac{1}{2}, 0, 0$	$\frac{1}{2}, 0, \frac{1}{2}$			$hkl : l = 2n$
2	<i>c</i> $\bar{1}$	$0, \frac{1}{2}, 0$	$0, \frac{1}{2}, \frac{1}{2}$			$hkl : l = 2n$
2	<i>b</i> $\bar{1}$	$\frac{1}{2}, \frac{1}{2}, 0$	$\frac{1}{2}, \frac{1}{2}, \frac{1}{2}$			$hkl : l = 2n$
2	<i>a</i> $\bar{1}$	$0, 0, 0$	$0, 0, \frac{1}{2}$			$hkl : l = 2n$

Symmetry of special projections

Along [001] $p2mm$
 $\mathbf{a}' = \mathbf{a}_p$ $\mathbf{b}' = \mathbf{b}$
Origin at 0, 0, z

Along [100] $p2gm$
 $\mathbf{a}' = \mathbf{b}$ $\mathbf{b}' = \mathbf{c}_p$
Origin at x, 0, 0

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

Maximal non-isomorphic subgroups

I [2] $P1c1$ (Pc , 7) 1; 4
[2] $P121$ ($P2$, 3) 1; 2
[2] $P\bar{1}$ (2) 1; 3

IIa none

IIb [2] $P12_1/c1$ ($\mathbf{b}' = 2\mathbf{b}$) ($P2_1/c$, 14); [2] $C12/c1$ ($\mathbf{a}' = 2\mathbf{a}, \mathbf{b}' = 2\mathbf{b}$) ($C2/c$, 15)

Maximal isomorphic subgroups of lowest index

IIc [2] $P12/c1$ ($\mathbf{b}' = 2\mathbf{b}$) ($P2/c$, 13); [2] $P12/c1$ ($\mathbf{a}' = 2\mathbf{a}$ or $\mathbf{a}' = 2\mathbf{a}, \mathbf{c}' = 2\mathbf{a} + \mathbf{c}$) ($P2/c$, 13)

Minimal non-isomorphic supergroups

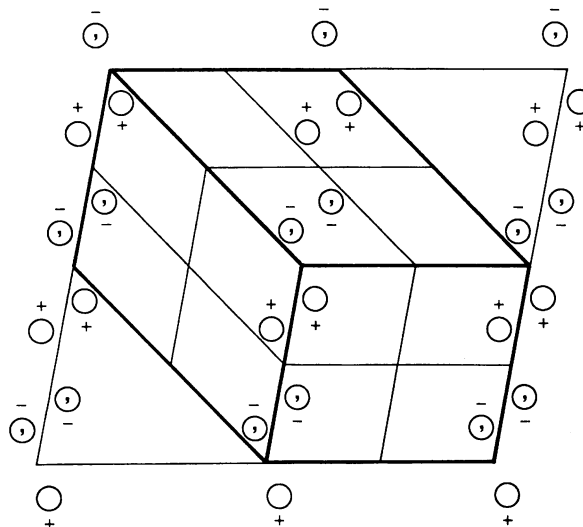
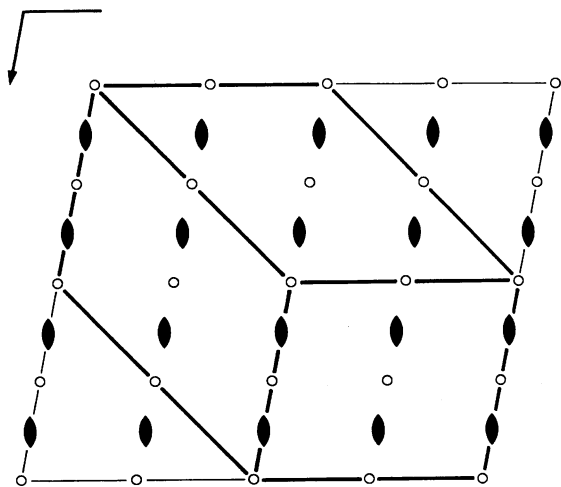
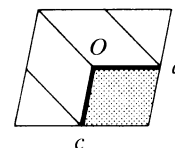
I [2] $Pnnn$ (48); [2] $Pccm$ (49); [2] $Pban$ (50); [2] $Pmma$ (51); [2] $Pnna$ (52); [2] $Pmna$ (53); [2] $Pcca$ (54); [2] $Pccn$ (56); [2] $Pbcm$ (57); [2] $Pmmn$ (59); [2] $Pbcn$ (60); [2] $Cmme$ (67); [2] $Ccce$ (68); [2] $P4/n$ (85); [2] $P4_2/n$ (86)

II [2] $A12/m1$ ($C2/m$, 12); [2] $C12/c1$ ($C2/c$, 15); [2] $I12/c1$ ($C2/c$, 15); [2] $P12/m1$ ($\mathbf{c}' = \frac{1}{2}\mathbf{c}$) ($P2/m$, 10)

$P2/c$ 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:

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

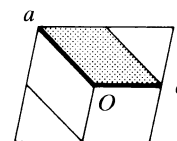
Special: as above, plus

no extra conditions

no extra conditions

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

P12/n1

UNIQUE AXIS b , CELL CHOICE 2Origin 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

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 b $\bar{1}$	$0, \frac{1}{2}, \frac{1}{2}$ $\frac{1}{2}, \frac{1}{2}, 0$
2 c $\bar{1}$	$0, \frac{1}{2}, 0$ $\frac{1}{2}, \frac{1}{2}, \frac{1}{2}$
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

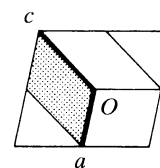
no extra conditions

no extra conditions

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

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

P12/a1

UNIQUE AXIS b , CELL CHOICE 3Origin 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

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 b $\bar{1}$	$\frac{1}{2}, \frac{1}{2}, \frac{1}{2}$ $0, \frac{1}{2}, \frac{1}{2}$
2 c $\bar{1}$	$0, \frac{1}{2}, 0$ $\frac{1}{2}, \frac{1}{2}, 0$
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

$2/m$

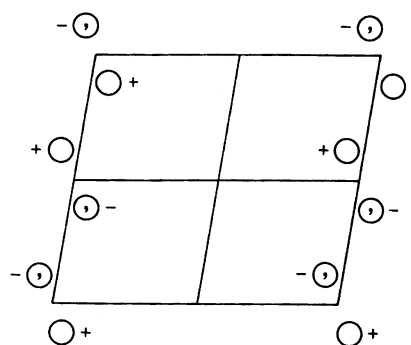
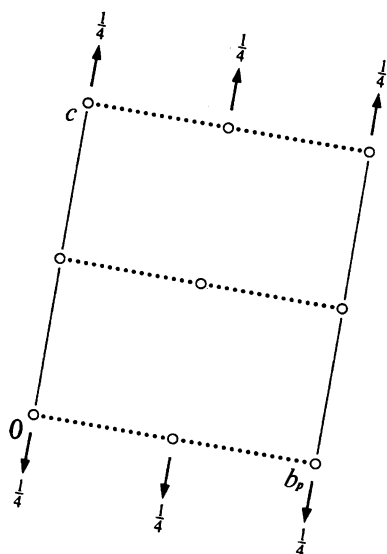
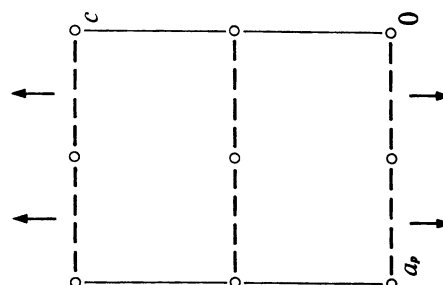
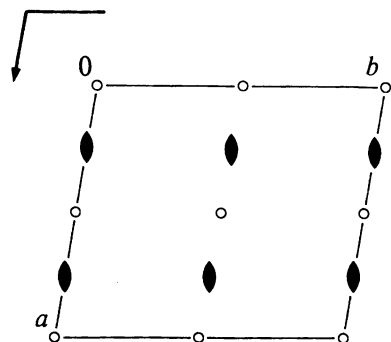
Monoclinic

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
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

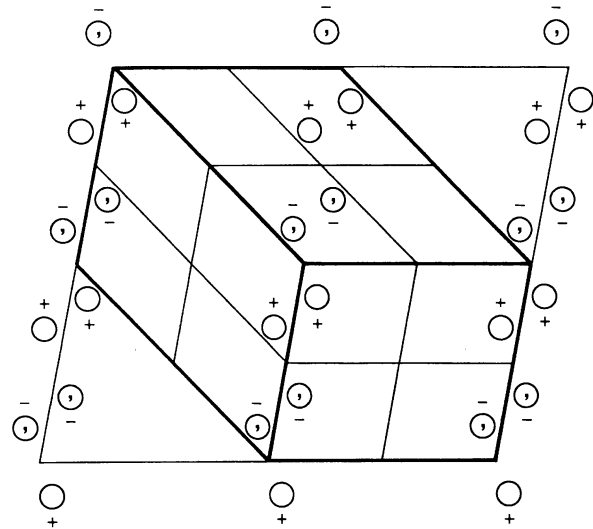
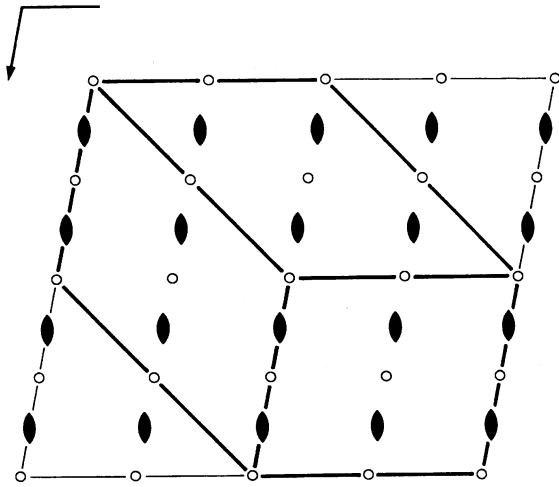
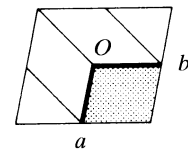
I [2] $Pnnn$ (48); [2] $Pccm$ (49); [2] $Pban$ (50); [2] $Pmma$ (51); [2] $Pnna$ (52); [2] $Pmna$ (53); [2] $Pcca$ (54); [2] $Pccn$ (56); [2] $Pbcm$ (57); [2] $Pmmn$ (59); [2] $Pbcn$ (60); [2] $Cmme$ (67); [2] $Ccce$ (68); [2] $P4/n$ (85); [2] $P4_2/n$ (86)

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

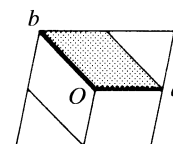
UNIQUE AXIS c , DIFFERENT CELL CHOICES $P112/a$ UNIQUE AXIS c , CELL CHOICE 1Origin at $\bar{1}$ on glide plane a Asymmetric unit $0 \leq x \leq \frac{1}{2}$; $0 \leq y \leq \frac{1}{2}$; $0 \leq z \leq 1$ Generators selected (1); $t(1,0,0)$; $t(0,1,0)$; $t(0,0,1)$; (2); (3)**Positions**Multiplicity,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

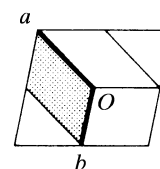
no extra conditions

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

$hkl : k = 2n$

$hkl : k = 2n$