

$P2_1/c$

C_{2h}^5

$2/m$

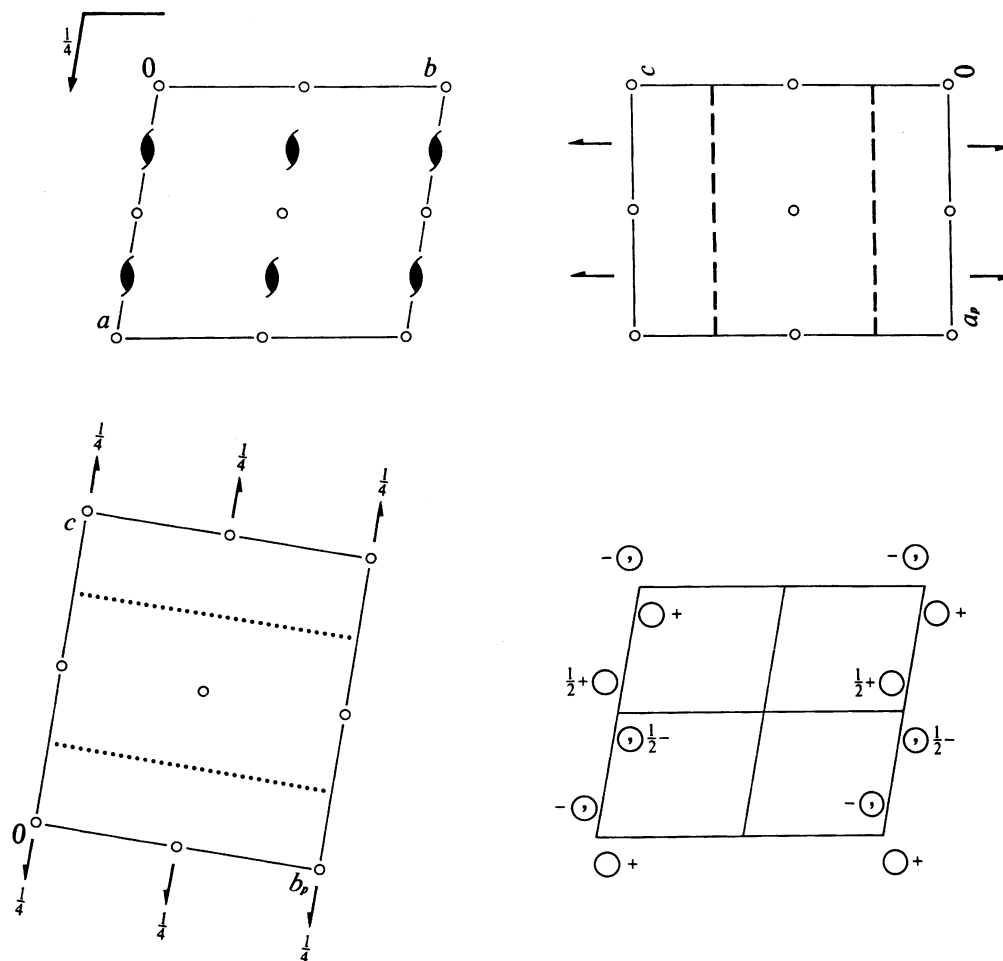
Monoclinic

No. 14

$P112_1/a$

Patterson symmetry $P112/m$

UNIQUE AXIS c , CELL CHOICE 1



Origin at $\bar{1}$

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

Symmetry operations

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

Generators selected (1); $t(1,0,0)$; $t(0,1,0)$; $t(0,0,1)$; (2); (3)

Positions

Multiplicity, Wyckoff letter, Site symmetry	Coordinates				Reflection conditions
					General:
4 <i>e</i> 1	(1) x, y, z	(2) $\bar{x} + \frac{1}{2}, \bar{y}, z + \frac{1}{2}$	(3) $\bar{x}, \bar{y}, \bar{z}$	(4) $x + \frac{1}{2}, y, \bar{z} + \frac{1}{2}$	$hk0 : h = 2n$ $00l : l = 2n$ $h00 : h = 2n$
					Special: as above, plus
2 <i>d</i> $\bar{1}$	$\frac{1}{2}, \frac{1}{2}, 0$	$0, \frac{1}{2}, \frac{1}{2}$			$hkl : h + l = 2n$
2 <i>c</i> $\bar{1}$	$\frac{1}{2}, 0, 0$	$0, 0, \frac{1}{2}$			$hkl : h + l = 2n$
2 <i>b</i> $\bar{1}$	$0, \frac{1}{2}, 0$	$\frac{1}{2}, \frac{1}{2}, \frac{1}{2}$			$hkl : h + l = 2n$
2 <i>a</i> $\bar{1}$	$0, 0, 0$	$\frac{1}{2}, 0, \frac{1}{2}$			$hkl : h + l = 2n$

Symmetry of special projections

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

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

Along $[010]$ $p2gg$
 $\mathbf{a}' = \mathbf{c}$ $\mathbf{b}' = \mathbf{a}_p$
 Origin at $0, y, 0$

Maximal non-isomorphic subgroups

I $[2] P11a (Pc, 7)$ 1; 4
 $[2] P112_1 (P2_1, 4)$ 1; 2
 $[2] P\bar{1} (2)$ 1; 3

IIa none

IIb none

Maximal isomorphic subgroups of lowest index

IIc $[2] P112_1/a (\mathbf{b}' = 2\mathbf{b} \text{ or } \mathbf{a}' = \mathbf{a} + 2\mathbf{b}, \mathbf{b}' = 2\mathbf{b}) (P2_1/c, 14)$; $[3] P112_1/a (\mathbf{c}' = 3\mathbf{c}) (P2_1/c, 14)$

Minimal non-isomorphic supergroups

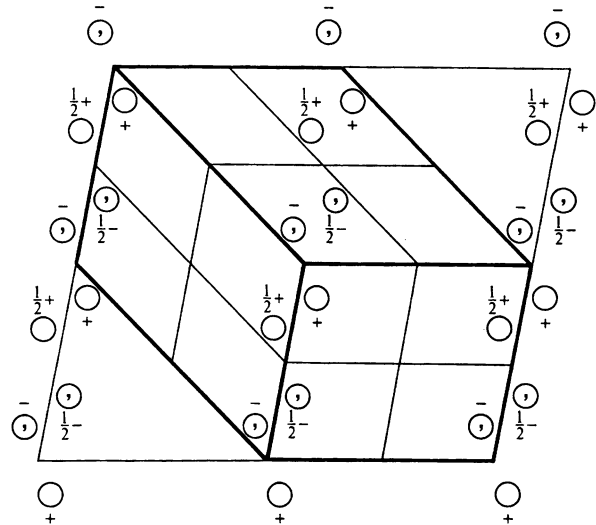
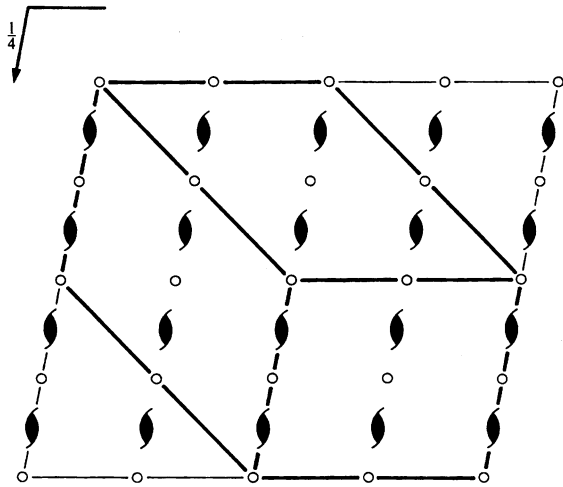
I $[2] Pnna (52)$; $[2] Pmna (53)$; $[2] Pcca (54)$; $[2] Pbam (55)$; $[2] Pccn (56)$; $[2] Pbcm (57)$; $[2] Pnnm (58)$; $[2] Pbcn (60)$;
 $[2] Pbca (61)$; $[2] Pnma (62)$; $[2] Cmce (64)$

II $[2] A112/a (C2/c, 15)$; $[2] B112/m (C2/m, 12)$; $[2] I112/a (C2/c, 15)$; $[2] P112_1/m (\mathbf{a}' = \frac{1}{2}\mathbf{a}) (P2_1/m, 11)$;
 $[2] P112/a (\mathbf{c}' = \frac{1}{2}\mathbf{c}) (P2/c, 13)$

$P2_1/c$ C_{2h}^5 $2/m$

Monoclinic

No. 14

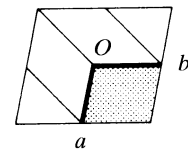
UNIQUE AXIS c , DIFFERENT CELL CHOICES $P112_1/a$ UNIQUE AXIS c , CELL CHOICE 1Origin at $\bar{1}$ Asymmetric unit $0 \leq x \leq 1; 0 \leq y \leq 1; 0 \leq z \leq \frac{1}{4}$ Generators selected (1); $t(1,0,0)$; $t(0,1,0)$; $t(0,0,1)$; (2); (3)

Positions

Multiplicity,
Wyckoff letter,
Site symmetry

Coordinates

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



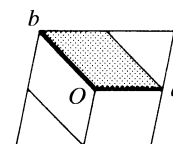
Reflection conditions

General:

 $hk0 : h = 2n$
 $00l : l = 2n$
 $h00 : h = 2n$

Special: as above, plus

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

$P112_1/n$ UNIQUE AXIS c , CELL CHOICE 2Origin at $\bar{1}$ 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	e	1	(1) x, y, z	(2) $\bar{x} + \frac{1}{2}, \bar{y} + \frac{1}{2}, z + \frac{1}{2}$	(3) $\bar{x}, \bar{y}, \bar{z}$	(4) $x + \frac{1}{2}, y + \frac{1}{2}, \bar{z} + \frac{1}{2}$
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Reflection conditions

General:

 $hk0 : h + k = 2n$ $00l : l = 2n$ $h00 : h = 2n$ $0k0 : k = 2n$

Special: as above, plus

2	d	$\bar{1}$	$0, \frac{1}{2}, 0$	$\frac{1}{2}, 0, \frac{1}{2}$
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 $hkl : h + k + l = 2n$

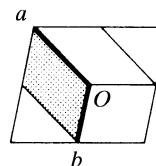
2	c	$\bar{1}$	$\frac{1}{2}, \frac{1}{2}, 0$	$0, 0, \frac{1}{2}$
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 $hkl : h + k + l = 2n$

2	b	$\bar{1}$	$\frac{1}{2}, 0, 0$	$0, \frac{1}{2}, \frac{1}{2}$
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 $hkl : h + k + l = 2n$

2	a	$\bar{1}$	$0, 0, 0$	$\frac{1}{2}, \frac{1}{2}, \frac{1}{2}$
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 $hkl : h + k + l = 2n$ $P112_1/b$ UNIQUE AXIS c , CELL CHOICE 3Origin at $\bar{1}$ 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	e	1	(1) x, y, z	(2) $\bar{x}, \bar{y} + \frac{1}{2}, z + \frac{1}{2}$	(3) $\bar{x}, \bar{y}, \bar{z}$	(4) $x, y + \frac{1}{2}, \bar{z} + \frac{1}{2}$
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Reflection conditions

General:

 $hk0 : k = 2n$ $00l : l = 2n$ $0k0 : k = 2n$

Special: as above, plus

2	d	$\bar{1}$	$\frac{1}{2}, 0, 0$	$\frac{1}{2}, \frac{1}{2}, \frac{1}{2}$
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 $hkl : k + l = 2n$

2	c	$\bar{1}$	$0, \frac{1}{2}, 0$	$0, 0, \frac{1}{2}$
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 $hkl : k + l = 2n$

2	b	$\bar{1}$	$\frac{1}{2}, \frac{1}{2}, 0$	$\frac{1}{2}, 0, \frac{1}{2}$
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 $hkl : k + l = 2n$

2	a	$\bar{1}$	$0, 0, 0$	$0, \frac{1}{2}, \frac{1}{2}$
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 $hkl : k + l = 2n$