

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

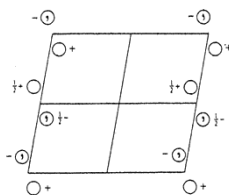
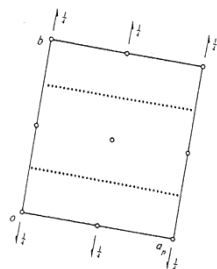
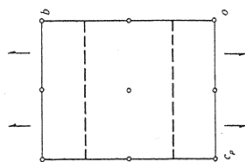
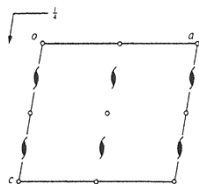
Monoclinic

CONTINUED

No. 14

 $P2_1/c$

No. 14

 $P12_1/c1$ Patterson symmetry $P12/m1$ UNIQUE AXIS b , CELL CHOICE 1Origin at $\bar{1}$ Asymmetric unit $0 \leq x \leq 1; 0 \leq y \leq \frac{1}{2}; 0 \leq z \leq 1$

Symmetry operations

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

General:

 $h0l: l = 2n$ $0k0: k = 2n$ $00l: l = 2n$

Special: as above, plus

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

Symmetry of special projections

Along [001] $p2gm$ $a' = a, b' = b$ Origin at $0, 0, z$ Along [100] $p2gg$ $a' = b, b' = c, c' = a$ Origin at $x, 0, 0$ Along [010] $p2$ $a' = \frac{1}{2}c, b' = a$ Origin at $0, y, 0$

Maximal non-isomorphic subgroups

I $[2]P12_1, 1(P2_1) 1; 2$ $[2]P\bar{1} 1; 3$ $[2]P1c1(Pc) 1; 4$

IIa none

IIb none

Maximal isomorphic subgroups of lowest index

IIc $[3]P12_1/c1(b' = 3b)(P2_1/c)$; $[2]P12_1/c1(a' = 2a \text{ or } a' = 2a, c' = 2a + c)(P2_1/c)$

Minimal non-isomorphic supergroups

I $[2]Pnna$; $[2]Pmna$; $[2]Pcca$; $[2]Pbam$; $[2]Pccn$; $[2]Pbcm$; $[2]Pnmm$; $[2]Pbcn$; $[2]Pbca$; $[2]Pnma$;
 $[2]Cmca$ II $[2]C12/c1(C2/c)$; $[2]A12/m1(C2/m)$; $[2]I12/c1(C2/c)$; $[2]P12_1/m1(2c' = c)(P2_1/m)$;
 $[2]P12/c1(2b' = b)(P2/c)$

$P 2_1/c$

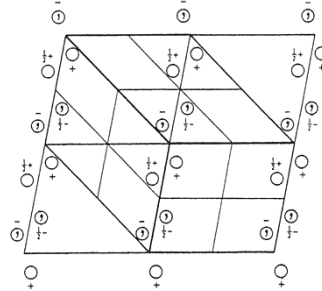
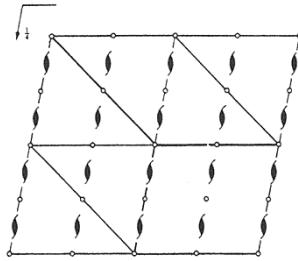
C_{2h}^5

$2/m$

Monoclinic

No. 14

UNIQUE AXIS b , DIFFERENT CELL CHOICES



$P 12_1/c 1$

UNIQUE AXIS b , CELL CHOICE 1



Origin at $\bar{1}$

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

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

2 d $\bar{1}$ $\frac{1}{2}, 0, \frac{1}{2}$ $\frac{1}{2}, \frac{1}{2}, 0$

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

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

Reflection conditions

General:

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

Special: as above, plus

$hkl: k+l=2n$

$hkl: k+l=2n$

$hkl: k+l=2n$

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No. 14

$P 2_1/c$

$P 12_1/n 1$

UNIQUE AXIS b , CELL CHOICE 2

Origin at $\bar{1}$

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

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

2 d $\bar{1}$ $\frac{1}{2}, 0, \frac{1}{2}$ $0, \frac{1}{2}, \frac{1}{2}$

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

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

2 a $\bar{1}$ $0, 0, 0$ $\frac{1}{2}, \frac{1}{2}, \frac{1}{2}$



Reflection conditions

General:

$h0l: h+l=2n$
 $0k0: k=2n$
 $h00: h=2n$
 $00l: l=2n$

Special: as above, plus

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

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

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

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

$P 12_1/a 1$

UNIQUE AXIS b , CELL CHOICE 3



Origin at $\bar{1}$

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

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

2 d $\bar{1}$ $0, 0, \frac{1}{2}$ $\frac{1}{2}, \frac{1}{2}, \frac{1}{2}$

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

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

Reflection conditions

General:

$h0l: h=2n$
 $0k0: k=2n$
 $h00: h=2n$

Special: as above, plus

$hkl: h+k=2n$

$hkl: h+k=2n$

$hkl: h+k=2n$