

*P*2

C_2^1

2

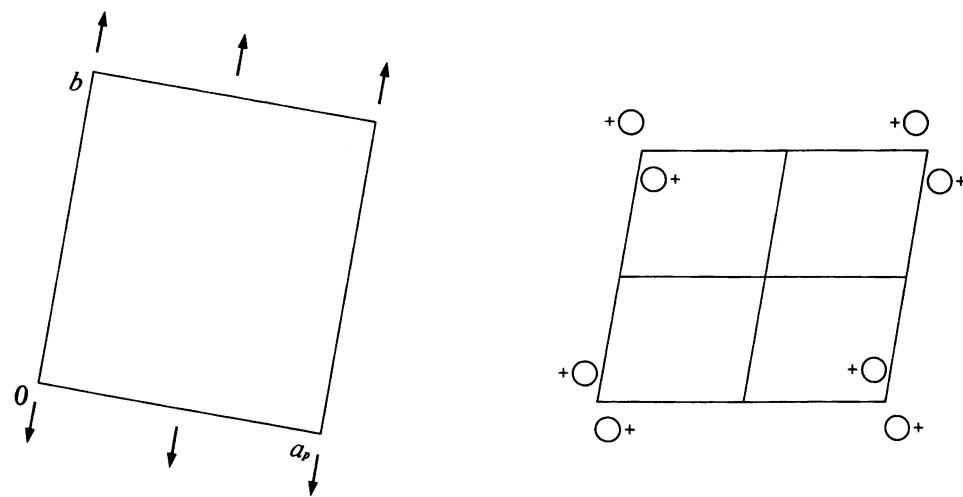
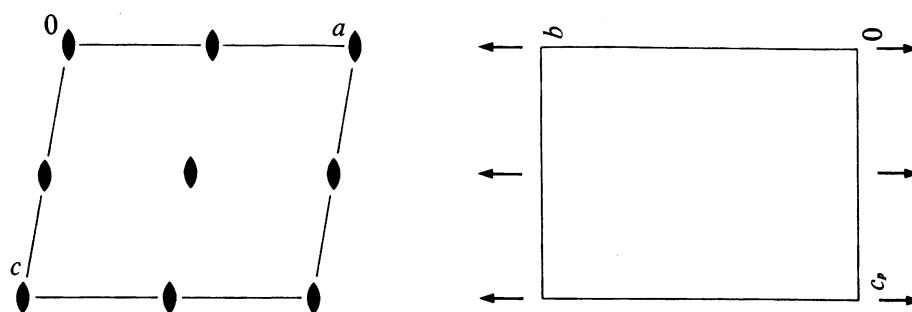
Monoclinic

No. 3

*P*121

Patterson symmetry *P*12/*m*1

UNIQUE AXIS *b*



Origin on 2

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

Symmetry operations

(1) 1 (2) 2 0, *y*, 0

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

Positions

Multiplicity, Wyckoff letter, Site symmetry	Coordinates	Reflection conditions
2 e 1	(1) x,y,z (2) \bar{x},y,\bar{z}	General: no conditions Special: no extra conditions
1 d 2	$\frac{1}{2},y,\frac{1}{2}$	
1 c 2	$\frac{1}{2},y,0$	
1 b 2	$0,y,\frac{1}{2}$	
1 a 2	$0,y,0$	

Symmetry of special projections

Along [001] $p\bar{1}m1$ $\mathbf{a}' = \mathbf{a}_p$ $\mathbf{b}' = \mathbf{b}$ Origin at $0,0,z$	Along [100] $p11m$ $\mathbf{a}' = \mathbf{b}$ $\mathbf{b}' = \mathbf{c}_p$ Origin at $x,0,0$	Along [010] $p2$ $\mathbf{a}' = \mathbf{c}$ $\mathbf{b}' = \mathbf{a}$ Origin at $0,y,0$
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Maximal non-isomorphic subgroups

I [2] $P1(1)$ 1		
IIa none		
IIb [2] $P12_11(\mathbf{b}' = 2\mathbf{b})(P2_1, 4)$; [2] $C121(\mathbf{a}' = 2\mathbf{a}, \mathbf{b}' = 2\mathbf{b})(C2, 5)$; [2] $A121(\mathbf{b}' = 2\mathbf{b}, \mathbf{c}' = 2\mathbf{c})(C2, 5)$; [2] $F121(\mathbf{a}' = 2\mathbf{a}, \mathbf{b}' = 2\mathbf{b}, \mathbf{c}' = 2\mathbf{c})(C2, 5)$		

Maximal isomorphic subgroups of lowest index

IIIc [2] $P121(\mathbf{b}' = 2\mathbf{b})(P2, 3)$; [2] $P121(\mathbf{c}' = 2\mathbf{c} \text{ or } \mathbf{a}' = 2\mathbf{a} \text{ or } \mathbf{a}' = \mathbf{a} + \mathbf{c}, \mathbf{c}' = -\mathbf{a} + \mathbf{c})(P2, 3)$
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Minimal non-isomorphic supergroups

I [2] $P2/m(10)$; [2] $P2/c(13)$; [2] $P222(16)$; [2] $P222_1(17)$; [2] $P2_12_12(18)$; [2] $C222(21)$; [2] $Pmm2(25)$; [2] $Pcc2(27)$; [2] $Pma2(28)$; [2] $Pnc2(30)$; [2] $Pba2(32)$; [2] $Pnn2(34)$; [2] $Cmm2(35)$; [2] $Ccc2(37)$; [2] $P4(75)$; [2] $P4_2(77)$; [2] $P\bar{4}(81)$; [3] $P6(168)$; [3] $P6_2(171)$; [3] $P6_4(172)$
II [2] $C121(C2, 5)$; [2] $A121(C2, 5)$; [2] $I121(C2, 5)$

*P*2

C_2^1

2

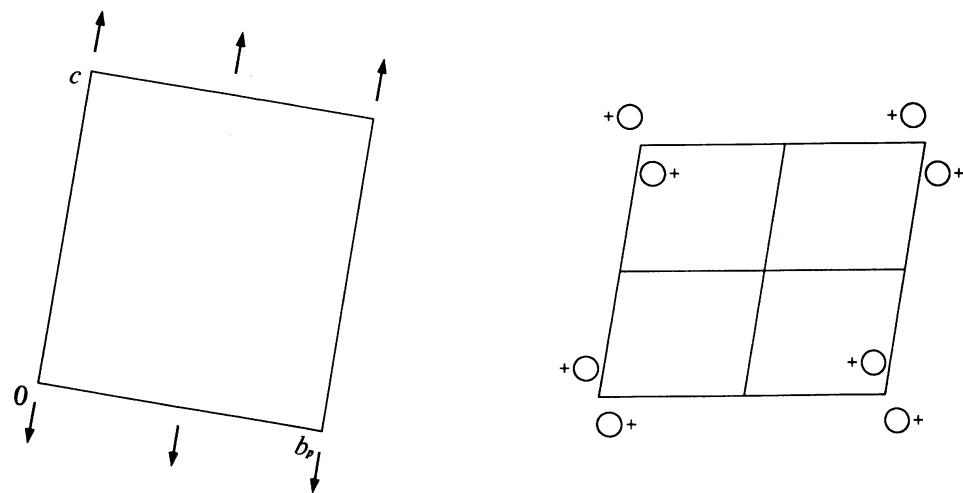
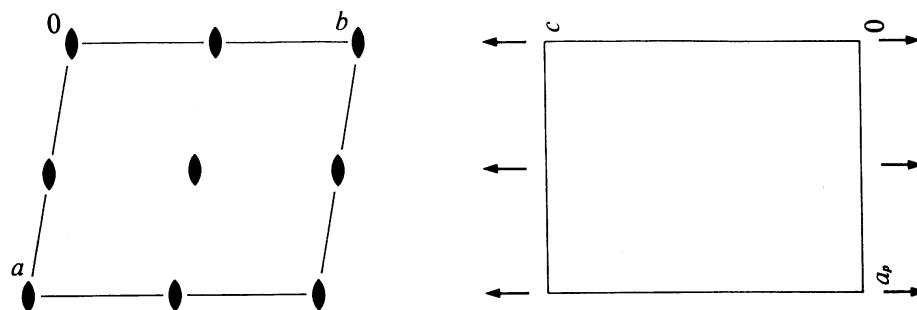
Monoclinic

No. 3

*P*112

Patterson symmetry *P*112/*m*

UNIQUE AXIS *c*



Origin on 2

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

Symmetry operations

(1) 1 (2) 2 0,0,*z*

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

Positions

Multiplicity, Wyckoff letter, Site symmetry	Coordinates	Reflection conditions
2 e 1	(1) x,y,z (2) \bar{x},\bar{y},z	General: no conditions Special: no extra conditions
1 d 2	$\frac{1}{2}, \frac{1}{2}, z$	
1 c 2	$0, \frac{1}{2}, z$	
1 b 2	$\frac{1}{2}, 0, z$	
1 a 2	$0, 0, z$	

Symmetry of special projections

Along [001] $p2$ $\mathbf{a}' = \mathbf{a}$ $\mathbf{b}' = \mathbf{b}$ Origin at $0,0,z$	Along [100] $p1m1$ $\mathbf{a}' = \mathbf{b}_p$ $\mathbf{b}' = \mathbf{c}$ Origin at $x,0,0$	Along [010] $p11m$ $\mathbf{a}' = \mathbf{c}$ $\mathbf{b}' = \mathbf{a}_p$ Origin at $0,y,0$
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Maximal non-isomorphic subgroups

I [2] $P1(1)$ 1		
IIa none		
IIb [2] $P112_1(\mathbf{c}' = 2\mathbf{c})(P2_1, 4)$; [2] $A112(\mathbf{b}' = 2\mathbf{b}, \mathbf{c}' = 2\mathbf{c})(C2, 5)$; [2] $B112(\mathbf{a}' = 2\mathbf{a}, \mathbf{c}' = 2\mathbf{c})(C2, 5)$; [2] $F112(\mathbf{a}' = 2\mathbf{a}, \mathbf{b}' = 2\mathbf{b}, \mathbf{c}' = 2\mathbf{c})(C2, 5)$		

Maximal isomorphic subgroups of lowest index

IIc [2] $P112(\mathbf{c}' = 2\mathbf{c})(P2, 3)$; [2] $P112(\mathbf{a}' = 2\mathbf{a} \text{ or } \mathbf{b}' = 2\mathbf{b} \text{ or } \mathbf{a}' = \mathbf{a} - \mathbf{b}, \mathbf{b}' = \mathbf{a} + \mathbf{b})(P2, 3)$
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Minimal non-isomorphic supergroups

I [2] $P2/m(10)$; [2] $P2/c(13)$; [2] $P222(16)$; [2] $P222_1(17)$; [2] $P2_12_12(18)$; [2] $C222(21)$; [2] $Pmm2(25)$; [2] $Pcc2(27)$; [2] $Pma2(28)$; [2] $Pnc2(30)$; [2] $Pba2(32)$; [2] $Pnn2(34)$; [2] $Cmm2(35)$; [2] $Ccc2(37)$; [2] $P4(75)$; [2] $P4_2(77)$; [2] $P\bar{4}(81)$; [3] $P6(168)$; [3] $P6_2(171)$; [3] $P6_4(172)$
II [2] $A112(C2, 5)$; [2] $B112(C2, 5)$; [2] $I112(C2, 5)$