

$Cc$

$C_s^4$

$m$

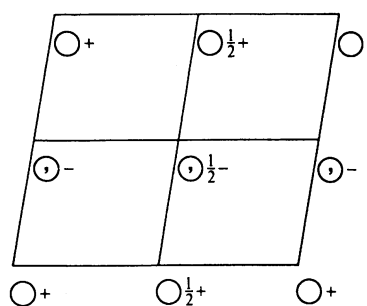
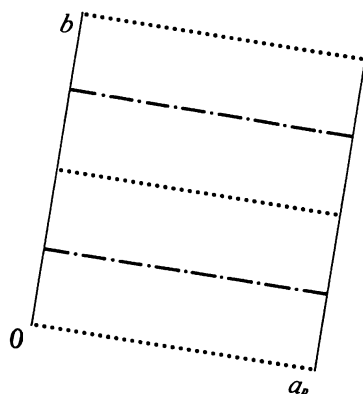
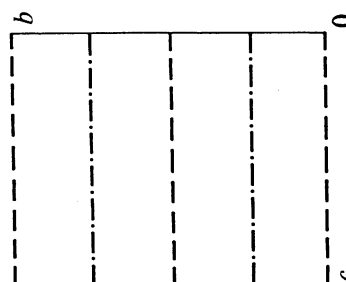
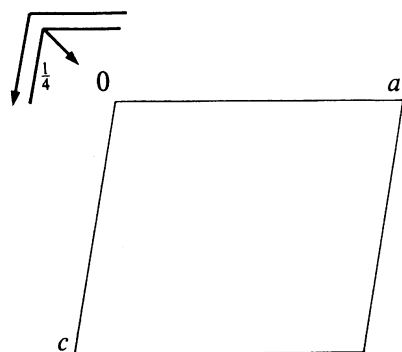
Monoclinic

No. 9

$C1c1$

Patterson symmetry  $C12/m1$

UNIQUE AXIS  $b$ , CELL CHOICE 1



**Origin** on glide plane  $c$

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

**Symmetry operations**

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

- (1) 1 (2)  $c \ x,0,z$

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

- (1)  $t(\frac{1}{2},\frac{1}{2},0)$  (2)  $n(\frac{1}{2},0,\frac{1}{2}) \ x,\frac{1}{4},z$

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

**Positions**

Multiplicity, Wyckoff letter, Site symmetry		Coordinates	Reflection conditions
		$(0,0,0)+$	General:
		$(\frac{1}{2},\frac{1}{2},0)+$	$hkl : h+k=2n$
4	<i>a</i> 1	(1) $x,y,z$	$h0l : h,l=2n$
		(2) $x,\bar{y},z+\frac{1}{2}$	$0kl : k=2n$
			$hk0 : h+k=2n$
			$0k0 : k=2n$
			$h00 : h=2n$
			$00l : l=2n$

**Symmetry of special projections**

Along [001]  $c11m$   
 $\mathbf{a}' = \mathbf{a}_p$      $\mathbf{b}' = \mathbf{b}$   
 Origin at  $0,0,z$

Along [100]  $p1g1$   
 $\mathbf{a}' = \frac{1}{2}\mathbf{b}$      $\mathbf{b}' = \mathbf{c}_p$   
 Origin at  $x,0,0$

Along [010]  $p1$   
 $\mathbf{a}' = \frac{1}{2}\mathbf{c}$      $\mathbf{b}' = \frac{1}{2}\mathbf{a}$   
 Origin at  $0,y,0$

**Maximal non-isomorphic subgroups**

- I** [2]  $C1(P1, 1)$  1+  
**IIa** [2]  $P1c1(Pc, 7)$  1; 2  
 [2]  $P1n1(Pc, 7)$  1;  $2 + (\frac{1}{2}, \frac{1}{2}, 0)$   
**IIb** none

**Maximal isomorphic subgroups of lowest index**

- IIc** [3]  $C1c1(\mathbf{b}' = 3\mathbf{b})(Cc, 9)$ ; [3]  $C1c1(\mathbf{c}' = 3\mathbf{c})(Cc, 9)$ ; [3]  $C1c1(\mathbf{a}' = 3\mathbf{a}$  or  $\mathbf{a}' = 3\mathbf{a}, \mathbf{c}' = -\mathbf{a} + \mathbf{c}$  or  $\mathbf{a}' = 3\mathbf{a}, \mathbf{c}' = \mathbf{a} + \mathbf{c})(Cc, 9)$

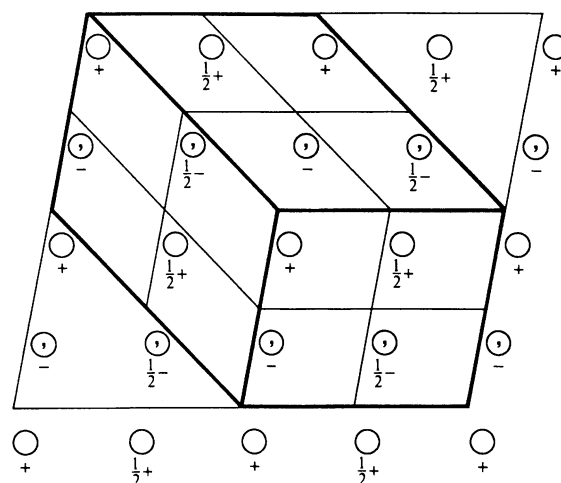
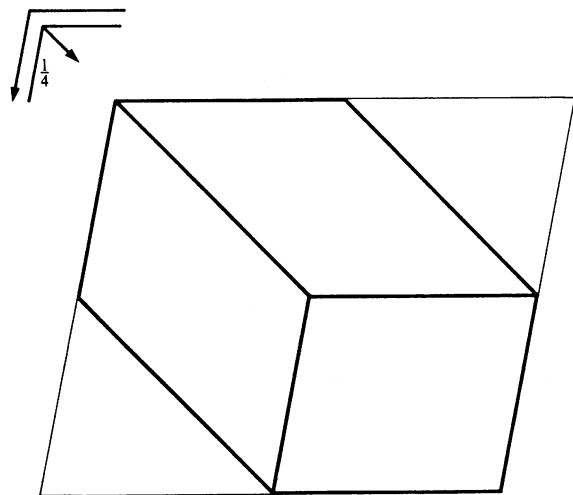
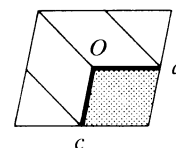
**Minimal non-isomorphic supergroups**

- I** [2]  $C2/c(15)$ ; [2]  $Cmc2_1(36)$ ; [2]  $Ccc2(37)$ ; [2]  $Ama2(40)$ ; [2]  $Aea2(41)$ ; [2]  $Fdd2(43)$ ; [2]  $Iba2(45)$ ; [2]  $Ima2(46)$ ;  
 [3]  $P3c1(158)$ ; [3]  $P31c(159)$ ; [3]  $R3c(161)$   
**II** [2]  $Fm1(Cm, 8)$ ; [2]  $C1m1(\mathbf{c}' = \frac{1}{2}\mathbf{c})(Cm, 8)$ ; [2]  $P1c1(\mathbf{a}' = \frac{1}{2}\mathbf{a}, \mathbf{b}' = \frac{1}{2}\mathbf{b})(Pc, 7)$

$Cc$  $C_s^4$  $m$ 

Monoclinic

No. 9

UNIQUE AXIS  $b$ , DIFFERENT CELL CHOICES $C1c1$ UNIQUE AXIS  $b$ , CELL CHOICE 1**Origin** on glide plane  $c$ **Asymmetric unit**  $0 \leq x \leq 1; 0 \leq y \leq \frac{1}{4}; 0 \leq z \leq 1$ **Generators selected** (1);  $t(1,0,0)$ ;  $t(0,1,0)$ ;  $t(0,0,1)$ ;  $t(\frac{1}{2}, \frac{1}{2}, 0)$ ; (2)**Positions**

Multiplicity, Wyckoff letter, Site symmetry	Coordinates
	$(0,0,0)+$ $(\frac{1}{2}, \frac{1}{2}, 0)+$

4	$a$	1	(1) $x, y, z$	(2) $x, \bar{y}, z + \frac{1}{2}$
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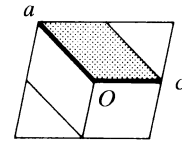
Reflection conditions

General:

 $hkl : h + k = 2n$  $h0l : h, l = 2n$  $0kl : k = 2n$  $hk0 : h + k = 2n$  $0k0 : k = 2n$  $h00 : h = 2n$  $00l : l = 2n$

**A1n1**UNIQUE AXIS  $b$ , CELL CHOICE 2**Origin** on glide plane  $n$ **Asymmetric unit**  $0 \leq x \leq 1; 0 \leq y \leq \frac{1}{4}; 0 \leq z \leq 1$ **Generators selected** (1);  $t(1,0,0)$ ;  $t(0,1,0)$ ;  $t(0,0,1)$ ;  $t(0, \frac{1}{2}, \frac{1}{2})$ ; (2)**Positions**

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



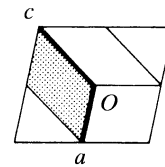
Reflection conditions

General:

$$\begin{aligned}
 hkl &: k + l = 2n \\
 h0l &: h, l = 2n \\
 0kl &: k + l = 2n \\
 hk0 &: k = 2n \\
 0k0 &: k = 2n \\
 h00 &: h = 2n \\
 00l &: l = 2n
 \end{aligned}$$

**I1a1**UNIQUE AXIS  $b$ , CELL CHOICE 3**Origin** on glide plane  $a$ **Asymmetric unit**  $0 \leq x \leq 1; 0 \leq y \leq \frac{1}{4}; 0 \leq z \leq 1$ **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)**Positions**

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



Reflection conditions

General:

$$\begin{aligned}
 hkl &: h + k + l = 2n \\
 h0l &: h, l = 2n \\
 0kl &: k + l = 2n \\
 hk0 &: h + k = 2n \\
 0k0 &: k = 2n \\
 h00 &: h = 2n \\
 00l &: l = 2n
 \end{aligned}$$

$Cc$ 

No. 9

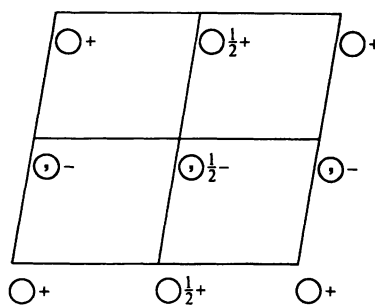
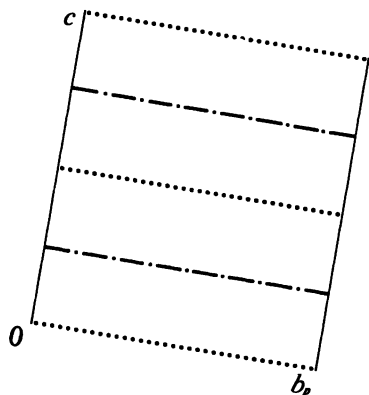
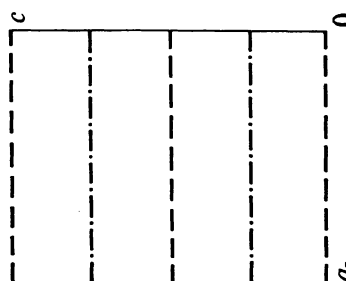
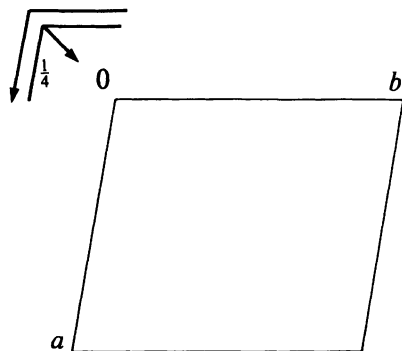
 $C_s^4$ 

A11a

 $m$ 

Monoclinic

Patterson symmetry A112/m

UNIQUE AXIS  $c$ , CELL CHOICE 1**Origin** on glide plane  $a$ **Asymmetric unit**  $0 \leq x \leq 1; 0 \leq y \leq 1; 0 \leq z \leq \frac{1}{4}$ **Symmetry operations**For  $(0, 0, 0)^+$  set(1) 1 (2)  $a$   $x, y, 0$ For  $(0, \frac{1}{2}, \frac{1}{2})^+$  set(1)  $t(0, \frac{1}{2}, \frac{1}{2})$  (2)  $n(\frac{1}{2}, \frac{1}{2}, 0)$   $x, y, \frac{1}{4}$

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

**Positions**

Multiplicity, Wyckoff letter, Site symmetry	Coordinates	Reflection conditions
	$(0,0,0)+ (0, \frac{1}{2}, \frac{1}{2})+$	<b>General:</b>
4 <i>a</i> 1	(1) $x,y,z$ (2) $x + \frac{1}{2}, y, \bar{z}$	$hkl : k + l = 2n$ $hk0 : h, k = 2n$ $0kl : k + l = 2n$ $h0l : l = 2n$ $00l : l = 2n$ $h00 : h = 2n$ $0k0 : k = 2n$

**Symmetry of special projections**

Along  $[001]$   $p1$   
 $\mathbf{a}' = \frac{1}{2}\mathbf{a}$   $\mathbf{b}' = \frac{1}{2}\mathbf{b}$   
 Origin at  $0,0,z$

Along  $[100]$   $c11m$   
 $\mathbf{a}' = \mathbf{b}_p$   $\mathbf{b}' = \mathbf{c}$   
 Origin at  $x,0,0$

Along  $[010]$   $p1g1$   
 $\mathbf{a}' = \frac{1}{2}\mathbf{c}$   $\mathbf{b}' = \mathbf{a}_p$   
 Origin at  $0,y,0$

**Maximal non-isomorphic subgroups**

- I**  $[2]A1(P1, 1)$   $1+$   
**IIa**  $[2]P11a(Pc, 7)$   $1; 2$   
 $[2]P11n(Pc, 7)$   $1; 2 + (0, \frac{1}{2}, \frac{1}{2})$   
**IIb** none

**Maximal isomorphic subgroups of lowest index**

- IIc**  $[3]A11a(\mathbf{c}' = 3\mathbf{c})(Cc, 9); [3]A11a(\mathbf{a}' = 3\mathbf{a})(Cc, 9); [3]A11a(\mathbf{b}' = 3\mathbf{b} \text{ or } \mathbf{a}' = \mathbf{a} - \mathbf{b}, \mathbf{b}' = 3\mathbf{b} \text{ or } \mathbf{a}' = \mathbf{a} + \mathbf{b}, \mathbf{b}' = 3\mathbf{b})(Cc, 9)$

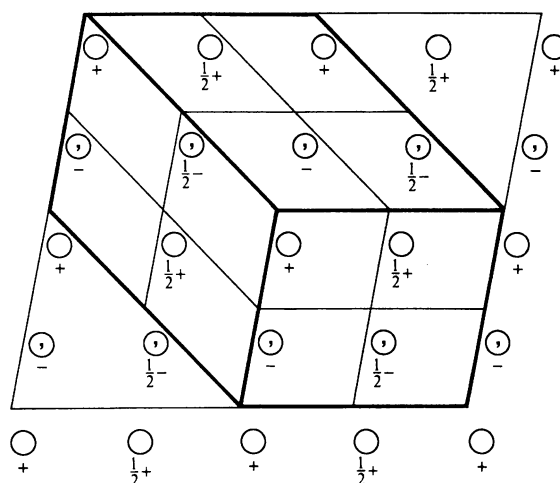
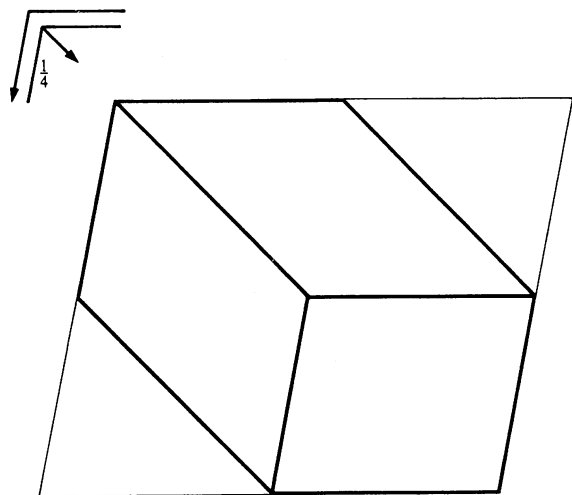
**Minimal non-isomorphic supergroups**

- I**  $[2]C2/c(15); [2]Cmc2_1(36); [2]Ccc2(37); [2]Ama2(40); [2]Aea2(41); [2]Fdd2(43); [2]Iba2(45); [2]Ima2(46); [3]P3c1(158); [3]P31c(159); [3]R3c(161)$   
**II**  $[2]F11m(Cm, 8); [2]A11m(\mathbf{a}' = \frac{1}{2}\mathbf{a})(Cm, 8); [2]P11a(\mathbf{b}' = \frac{1}{2}\mathbf{b}, \mathbf{c}' = \frac{1}{2}\mathbf{c})(Pc, 7)$

$Cc$  $C_s^4$  $m$ 

Monoclinic

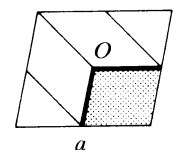
No. 9

UNIQUE AXIS  $c$ , DIFFERENT CELL CHOICES $A11a$ UNIQUE AXIS  $c$ , CELL CHOICE 1Origin on glide plane  $a$ Asymmetric unit  $0 \leq x \leq 1; 0 \leq y \leq 1; 0 \leq z \leq \frac{1}{4}$ Generators selected (1);  $t(1,0,0)$ ;  $t(0,1,0)$ ;  $t(0,0,1)$ ;  $t(0, \frac{1}{2}, \frac{1}{2})$ ; (2)

Positions

Multiplicity, Wyckoff letter, Site symmetry	Coordinates
	$(0,0,0)+ (0, \frac{1}{2}, \frac{1}{2})+$

4	$a$	1	(1) $x,y,z$	(2) $x + \frac{1}{2}, y, \bar{z}$
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Reflection conditions

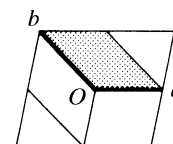
General:

 $hkl : k + l = 2n$  $hk0 : h, k = 2n$  $0kl : k + l = 2n$  $h0l : l = 2n$  $00l : l = 2n$  $h00 : h = 2n$  $0k0 : k = 2n$

**B11n**UNIQUE AXIS  $c$ , CELL CHOICE 2**Origin** 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);  $t(1,0,0)$ ;  $t(0,1,0)$ ;  $t(0,0,1)$ ;  $t(\frac{1}{2},0,\frac{1}{2})$ ; (2)**Positions**

Multiplicity, Wyckoff letter, Site symmetry	Coordinates
	$(0,0,0) + (\frac{1}{2},0,\frac{1}{2}) +$

4	$a$	1	(1) $x,y,z$	(2) $x + \frac{1}{2}, y + \frac{1}{2}, \bar{z}$
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Reflection conditions

General:

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

$$hk0 : h, k = 2n$$

$$0kl : l = 2n$$

$$h0l : h + l = 2n$$

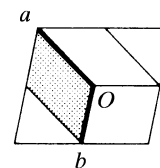
$$00l : l = 2n$$

$$h00 : h = 2n$$

$$0k0 : k = 2n$$
**I11b**UNIQUE AXIS  $c$ , CELL CHOICE 3**Origin** on glide plane  $b$ **Asymmetric unit**  $0 \leq x \leq 1; 0 \leq y \leq 1; 0 \leq z \leq \frac{1}{4}$ **Generators selected** (1);  $t(1,0,0)$ ;  $t(0,1,0)$ ;  $t(0,0,1)$ ;  $t(\frac{1}{2},\frac{1}{2},\frac{1}{2})$ ; (2)**Positions**

Multiplicity, Wyckoff letter, Site symmetry	Coordinates
	$(0,0,0) + (\frac{1}{2},\frac{1}{2},\frac{1}{2}) +$

4	$a$	1	(1) $x,y,z$	(2) $x,y + \frac{1}{2}, \bar{z}$
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Reflection conditions

General:

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

$$hk0 : h, k = 2n$$

$$0kl : k + l = 2n$$

$$h0l : h + l = 2n$$

$$00l : l = 2n$$

$$h00 : h = 2n$$

$$0k0 : k = 2n$$