

$C2/c$

$C_{2h}^6$

$2/m$

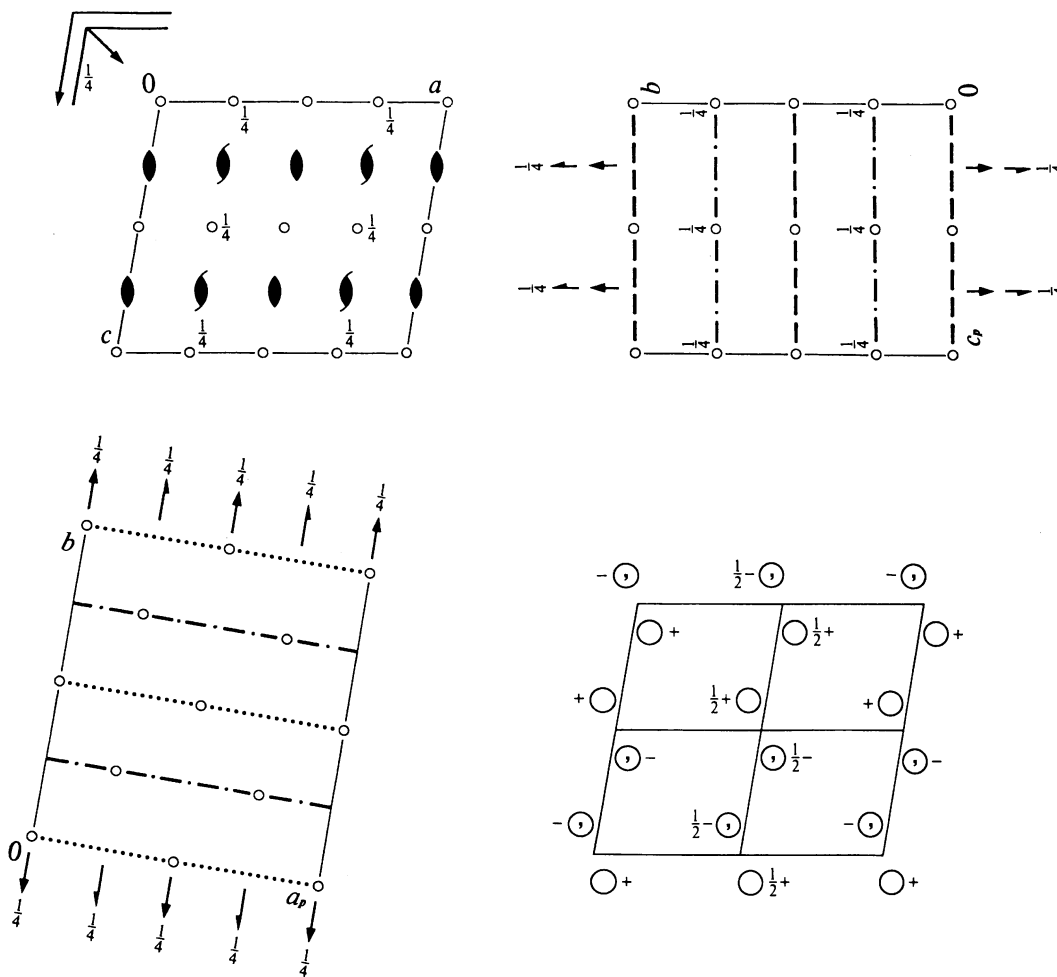
Monoclinic

No. 15

$C12/c1$

Patterson symmetry  $C12/m1$

UNIQUE AXIS  $b$ , CELL CHOICE 1



Origin at  $\bar{1}$  on glide plane  $c$

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

Symmetry operations

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

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

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

- |                                      |  |   |  |
|--------------------------------------|--|---|--|
| (1) $t(\frac{1}{2}, \frac{1}{2}, 0)$ | (2) $2(0, \frac{1}{2}, 0) \quad \frac{1}{4}, y, \frac{1}{4}$ | (3) $\bar{1} \quad \frac{1}{4}, \frac{1}{4}, 0$ | (4) $n(\frac{1}{2}, 0, \frac{1}{2}) \quad x, \frac{1}{4}, z$ |
|--------------------------------------|--|---|--|

**Generators selected** (1);  $t(1,0,0)$ ;  $t(0,1,0)$ ;  $t(0,0,1)$ ;  $t(\frac{1}{2},\frac{1}{2},0)$ ; (2); (3)

**Positions**

Multiplicity, Wyckoff letter, Site symmetry	Coordinates				Reflection conditions
	$(0,0,0)+ (\frac{1}{2},\frac{1}{2},0)+$				General:
8 <i>f</i> 1	(1) $x,y,z$	(2) $\bar{x},y,\bar{z}+\frac{1}{2}$	(3) $\bar{x},\bar{y},\bar{z}$	(4) $x,\bar{y},z+\frac{1}{2}$	$hkl : h+k=2n$ $h0l : h,l=2n$ $0kl : k=2n$ $hk0 : h+k=2n$ $0k0 : k=2n$ $h00 : h=2n$ $00l : l=2n$
					Special: as above, plus
4 <i>e</i> 2	$0,y,\frac{1}{4}$	$0,\bar{y},\frac{3}{4}$			no extra conditions
4 <i>d</i> $\bar{1}$	$\frac{1}{4},\frac{1}{4},\frac{1}{2}$	$\frac{3}{4},\frac{1}{4},0$			$hkl : k+l=2n$
4 <i>c</i> $\bar{1}$	$\frac{1}{4},\frac{1}{4},0$	$\frac{3}{4},\frac{1}{4},\frac{1}{2}$			$hkl : k+l=2n$
4 <i>b</i> $\bar{1}$	$0,\frac{1}{2},0$	$0,\frac{1}{2},\frac{1}{2}$			$hkl : l=2n$
4 <i>a</i> $\bar{1}$	$0,0,0$	$0,0,\frac{1}{2}$			$hkl : l=2n$

**Symmetry of special projections**

Along [001]  $c2mm$   
 $\mathbf{a}' = \mathbf{a}_p$      $\mathbf{b}' = \mathbf{b}$   
 Origin at 0,0,z

Along [100]  $p2gm$   
 $\mathbf{a}' = \frac{1}{2}\mathbf{b}$      $\mathbf{b}' = \mathbf{c}_p$   
 Origin at x,0,0

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

**Maximal non-isomorphic subgroups**

<b>I</b>	[2] $C1c1$ ( $Cc$ , 9)	(1; 4)+
	[2] $C121$ ( $C2$ , 5)	(1; 2)+
	[2] $C\bar{1}$ ( $P\bar{1}$ , 2)	(1; 3)+
<b>IIa</b>	[2] $P12_1/n1$ ( $P2_1/c$ , 14)	1; 3; (2; 4) + $(\frac{1}{2},\frac{1}{2},0)$
	[2] $P12_1/c1$ ( $P2_1/c$ , 14)	1; 4; (2; 3) + $(\frac{1}{2},\frac{1}{2},0)$
	[2] $P12/c1$ ( $P2/c$ , 13)	1; 2; 3; 4
	[2] $P12/n1$ ( $P2/c$ , 13)	1; 2; (3; 4) + $(\frac{1}{2},\frac{1}{2},0)$
<b>IIb</b>	none	

**Maximal isomorphic subgroups of lowest index**

**IIc** [3]  $C12/c1$  ( $\mathbf{b}' = 3\mathbf{b}$ ) ( $C2/c$ , 15); [3]  $C12/c1$  ( $\mathbf{c}' = 3\mathbf{c}$ ) ( $C2/c$ , 15);  
 [3]  $C12/c1$  ( $\mathbf{a}' = 3\mathbf{a}$  or  $\mathbf{a}' = 3\mathbf{a}, \mathbf{c}' = -\mathbf{a} + \mathbf{c}$  or  $\mathbf{a}' = 3\mathbf{a}, \mathbf{c}' = \mathbf{a} + \mathbf{c}$ ) ( $C2/c$ , 15)

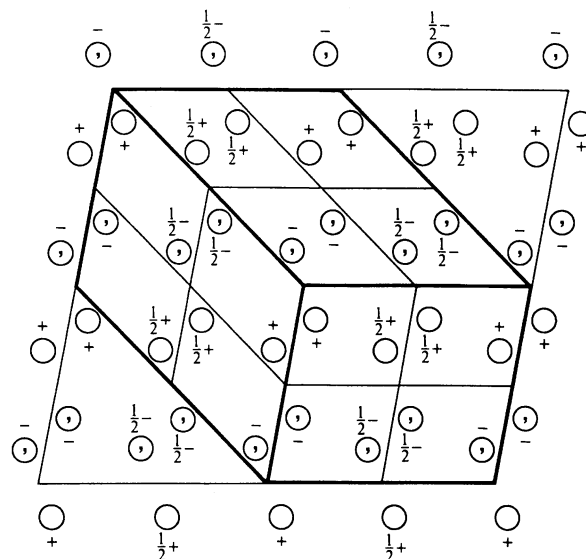
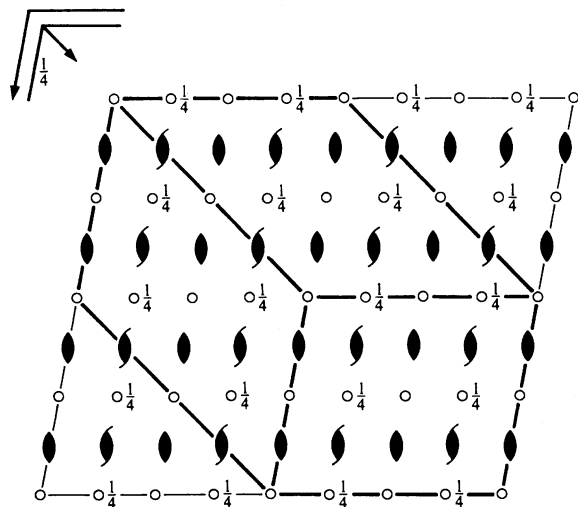
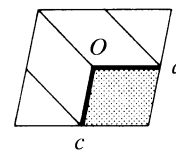
**Minimal non-isomorphic supergroups**

<b>I</b>	[2] $Cmcm$ (63); [2] $Cmce$ (64); [2] $Cccm$ (66); [2] $Ccce$ (68); [2] $Fddd$ (70); [2] $Ibam$ (72); [2] $Ibca$ (73); [2] $Imma$ (74); [2] $I4_1/a$ (88); [3] $P\bar{3}1c$ (163); [3] $P\bar{3}c1$ (165); [3] $R\bar{3}c$ (167)
<b>II</b>	[2] $F12/m1$ ( $C2/m$ , 12); [2] $C12/m1$ ( $\mathbf{c}' = \frac{1}{2}\mathbf{c}$ ) ( $C2/m$ , 12); [2] $P12/c1$ ( $\mathbf{a}' = \frac{1}{2}\mathbf{a}, \mathbf{b}' = \frac{1}{2}\mathbf{b}$ ) ( $P2/c$ , 13)

$C2/c$  $C_{2h}^6$  $2/m$ 

Monoclinic

No. 15

UNIQUE AXIS  $b$ , DIFFERENT CELL CHOICES $C12/c1$ UNIQUE AXIS  $b$ , CELL CHOICE 1Origin at  $\bar{1}$  on glide plane  $c$ Asymmetric unit  $0 \leq x \leq \frac{1}{2}$ ;  $0 \leq y \leq \frac{1}{2}$ ;  $0 \leq z \leq \frac{1}{2}$ Generators selected (1);  $t(1,0,0)$ ;  $t(0,1,0)$ ;  $t(0,0,1)$ ;  $t(\frac{1}{2}, \frac{1}{2}, 0)$ ; (2); (3)**Positions**Multiplicity,  
Wyckoff letter,  
Site symmetry

Coordinates

Reflection conditions

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

General:

8  $f$  1 (1)  $x,y,z$  (2)  $\bar{x},y,\bar{z}+\frac{1}{2}$  (3)  $\bar{x},\bar{y},\bar{z}$  (4)  $x,\bar{y},z+\frac{1}{2}$ 
 $hkl : h+k=2n$        $0k0 : k=2n$   
 $h0l : h,l=2n$        $h00 : h=2n$   
 $0kl : k=2n$        $00l : l=2n$   
 $hk0 : h+k=2n$ 

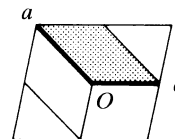
Special: as above, plus

4  $e$  2  $0,y,\frac{1}{4}$   $0,\bar{y},\frac{3}{4}$ 

no extra conditions

4  $d$   $\bar{1}$   $\frac{1}{4},\frac{1}{4},\frac{1}{2}$   $\frac{3}{4},\frac{3}{4},0$  4  $c$   $\bar{1}$   $\frac{1}{4},\frac{1}{4},0$   $\frac{3}{4},\frac{1}{4},\frac{1}{2}$  $hkl : k+l=2n$ 4  $b$   $\bar{1}$   $0,\frac{1}{2},0$   $0,\frac{1}{2},\frac{1}{2}$  4  $a$   $\bar{1}$   $0,0,0$   $0,0,\frac{1}{2}$  $hkl : l=2n$

## A12/n1

UNIQUE AXIS  $b$ , CELL CHOICE 2**Origin** at  $\bar{1}$  on glide plane  $n$ **Asymmetric unit**  $0 \leq x \leq \frac{1}{2}$ ;  $0 \leq y \leq 1$ ;  $0 \leq z \leq \frac{1}{4}$ **Generators selected** (1);  $t(1,0,0)$ ;  $t(0,1,0)$ ;  $t(0,0,1)$ ;  $t(0, \frac{1}{2}, \frac{1}{2})$ ; (2); (3)**Positions**Multiplicity,  
Wyckoff letter,  
Site symmetry

Coordinates

Reflection conditions

(0,0,0)+

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

General:

8  $f$  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)  $x + \frac{1}{2}, \bar{y}, z + \frac{1}{2}$ 
 $hkl : k + l = 2n$        $0k0 : k = 2n$   
 $h0l : h, l = 2n$        $h00 : h = 2n$   
 $0kl : k + l = 2n$        $00l : l = 2n$   
 $hk0 : k = 2n$ 

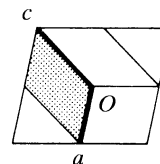
Special: as above, plus

4  $e$  2  $\frac{3}{4}, y, \frac{3}{4}$   $\frac{1}{4}, \bar{y}, \frac{1}{4}$ 

no extra conditions

4  $d$   $\bar{1}$   $\frac{1}{2}, \frac{1}{4}, \frac{3}{4}$   $0, \frac{1}{4}, \frac{3}{4}$  4  $c$   $\bar{1}$   $0, \frac{1}{4}, \frac{1}{4}$   $\frac{1}{2}, \frac{1}{4}, \frac{1}{4}$  $hkl : h = 2n$ 4  $b$   $\bar{1}$   $0, \frac{1}{2}, 0$   $\frac{1}{2}, \frac{1}{2}, \frac{1}{2}$  4  $a$   $\bar{1}$   $0, 0, 0$   $\frac{1}{2}, 0, \frac{1}{2}$  $hkl : h + k = 2n$ 

## I12/a1

UNIQUE AXIS  $b$ , CELL CHOICE 3**Origin** at  $\bar{1}$  on glide plane  $a$ **Asymmetric unit**  $0 \leq x \leq 1$ ;  $0 \leq y \leq \frac{1}{2}$ ;  $0 \leq z \leq \frac{1}{4}$ **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); (3)**Positions**Multiplicity,  
Wyckoff letter,  
Site symmetry

Coordinates

Reflection conditions

(0,0,0)+

 $(\frac{1}{2}, \frac{1}{2}, \frac{1}{2})+$ 

General:

8  $f$  1 (1)  $x, y, z$  (2)  $\bar{x} + \frac{1}{2}, y, \bar{z}$  (3)  $\bar{x}, \bar{y}, \bar{z}$  (4)  $x + \frac{1}{2}, \bar{y}, z$ 
 $hkl : h + k + l = 2n$        $0k0 : k = 2n$   
 $h0l : h, l = 2n$        $h00 : h = 2n$   
 $0kl : k + l = 2n$        $00l : l = 2n$   
 $hk0 : h + k = 2n$ 

Special: as above, plus

4  $e$  2  $\frac{1}{4}, y, 0$   $\frac{3}{4}, \bar{y}, 0$ 

no extra conditions

4  $d$   $\bar{1}$   $\frac{1}{4}, \frac{1}{4}, \frac{3}{4}$   $\frac{1}{4}, \frac{1}{4}, \frac{1}{4}$  4  $c$   $\bar{1}$   $\frac{3}{4}, \frac{1}{4}, \frac{3}{4}$   $\frac{3}{4}, \frac{1}{4}, \frac{1}{4}$  $hkl : l = 2n$ 4  $b$   $\bar{1}$   $0, \frac{1}{2}, 0$   $\frac{1}{2}, \frac{1}{2}, 0$  4  $a$   $\bar{1}$   $0, 0, 0$   $\frac{1}{2}, 0, 0$  $hkl : h = 2n$