

$P2_1/c$

$C_{2h}^5$

$2/m$

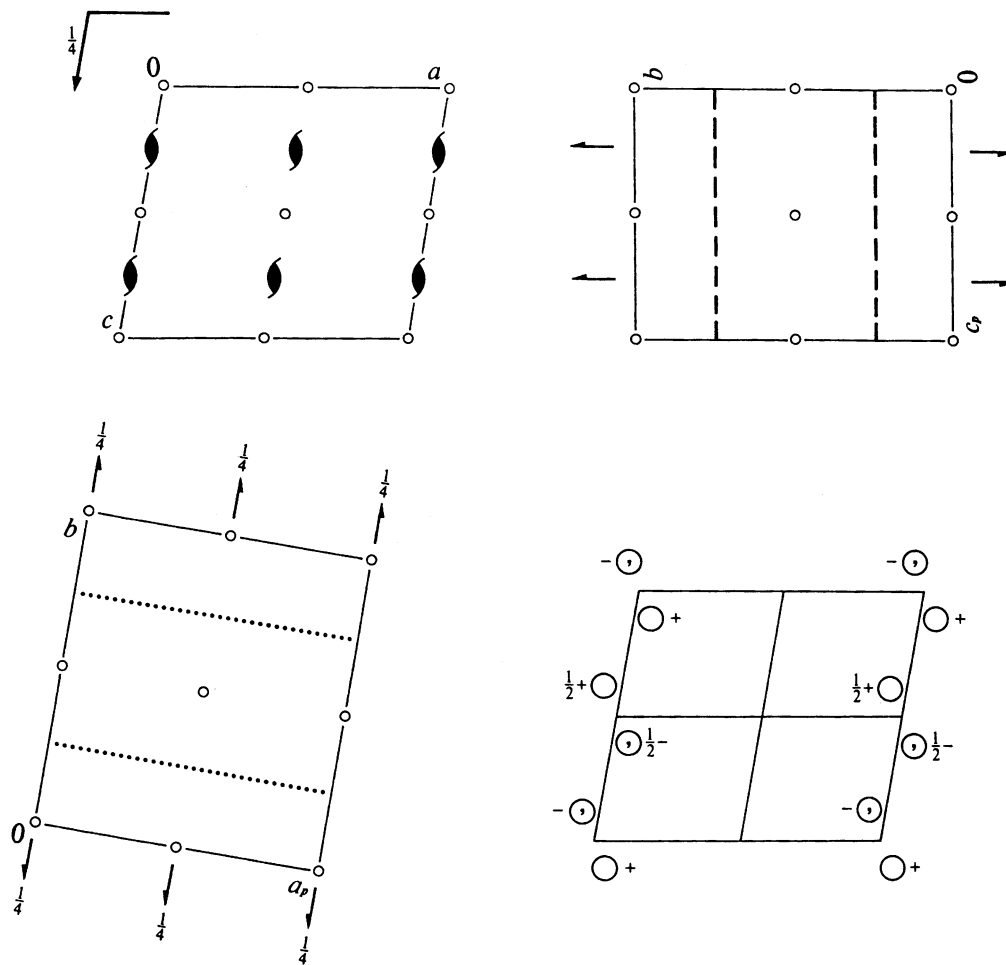
Monoclinic

No. 14

$P12_1/c1$

Patterson symmetry  $P12/m1$

UNIQUE AXIS  $b$ , CELL CHOICE 1



Origin at  $\bar{1}$

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

Symmetry operations

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

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

**Positions**

| Multiplicity,<br>Wyckoff letter,<br>Site symmetry | Coordinates                   |   |                                 |   | Reflection conditions   |
|---|-------------------------------|---|---------------------------------|---|---|
| 4 <i>e</i> 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:<br>$h0l : l = 2n$<br>$0k0 : k = 2n$<br>$00l : l = 2n$<br>Special: as above, plus<br>$hkl : k + l = 2n$ |
| 2 <i>d</i> $\bar{1}$                              | $\frac{1}{2}, 0, \frac{1}{2}$ | $\frac{1}{2}, \frac{1}{2}, 0$                         |                                 |   | $hkl : k + l = 2n$  |
| 2 <i>c</i> $\bar{1}$                              | $0, 0, \frac{1}{2}$           | $0, \frac{1}{2}, 0$                                   |                                 |   | $hkl : k + l = 2n$  |
| 2 <i>b</i> $\bar{1}$                              | $\frac{1}{2}, 0, 0$           | $\frac{1}{2}, \frac{1}{2}, \frac{1}{2}$               |                                 |   | $hkl : k + l = 2n$  |
| 2 <i>a</i> $\bar{1}$                              | $0, 0, 0$                     | $0, \frac{1}{2}, \frac{1}{2}$                         |                                 |   | $hkl : k + l = 2n$  |

**Symmetry of special projections**

Along  $[001]$   $p2gm$

$\mathbf{a}' = \mathbf{a}_p$      $\mathbf{b}' = \mathbf{b}$

Origin at  $0, 0, z$

Along  $[100]$   $p2gg$

$\mathbf{a}' = \mathbf{b}$      $\mathbf{b}' = \mathbf{c}_p$

Origin at  $x, 0, 0$

Along  $[010]$   $p2$

$\mathbf{a}' = \frac{1}{2}\mathbf{c}$      $\mathbf{b}' = \mathbf{a}$

Origin at  $0, y, 0$

**Maximal non-isomorphic subgroups**

**I**     $[2] P1c1 (Pc, 7)$     1; 4  
        $[2] P12_11 (P2_1, 4)$     1; 2  
        $[2] P\bar{1} (2)$     1; 3

**IIa** none

**IIb** none

**Maximal isomorphic subgroups of lowest index**

**IIc**     $[2] P12_1/c1 (\mathbf{a}' = 2\mathbf{a}$  or  $\mathbf{a}' = 2\mathbf{a}, \mathbf{c}' = 2\mathbf{a} + \mathbf{c}) (P2_1/c, 14)$ ;  $[3] P12_1/c1 (\mathbf{b}' = 3\mathbf{b}) (P2_1/c, 14)$

**Minimal non-isomorphic supergroups**

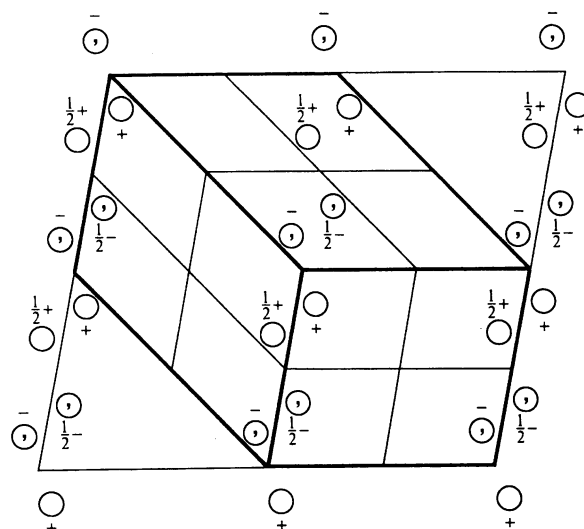
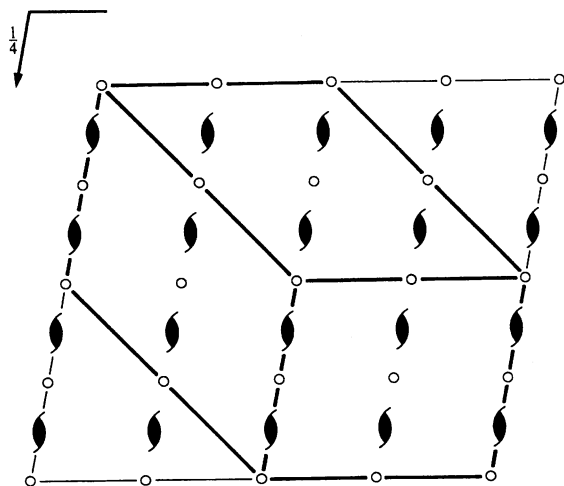
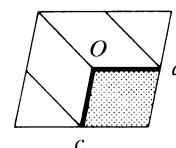
**I**     $[2] Pnna (52)$ ;  $[2] Pmna (53)$ ;  $[2] Pcca (54)$ ;  $[2] Pbam (55)$ ;  $[2] Pccn (56)$ ;  $[2] Pbcm (57)$ ;  $[2] Pnnm (58)$ ;  $[2] Pbcn (60)$ ;  
        $[2] Pbca (61)$ ;  $[2] Pnma (62)$ ;  $[2] Cmce (64)$

**II**     $[2] A12/m1 (C2/m, 12)$ ;  $[2] C12/c1 (C2/c, 15)$ ;  $[2] I12/c1 (C2/c, 15)$ ;  $[2] P12_1/m1 (\mathbf{c}' = \frac{1}{2}\mathbf{c}) (P2_1/m, 11)$ ;  
        $[2] P12/c1 (\mathbf{b}' = \frac{1}{2}\mathbf{b}) (P2/c, 13)$

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

Monoclinic

No. 14

UNIQUE AXIS  $b$ , DIFFERENT CELL CHOICES $P12_1/c1$ UNIQUE AXIS  $b$ , CELL CHOICE 1Origin at  $\bar{1}$ Asymmetric unit  $0 \leq x \leq 1$ ;  $0 \leq y \leq \frac{1}{4}$ ;  $0 \leq z \leq 1$ Generators selected (1);  $t(1,0,0)$ ;  $t(0,1,0)$ ;  $t(0,0,1)$ ; (2); (3)

Positions

Multiplicity,  
Wyckoff letter,  
Site symmetry

Coordinates

| Multiplicity,<br>Wyckoff letter,<br>Site symmetry | Coordinates   |
|---|---|
| 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) $x, \bar{y} + \frac{1}{2}, z + \frac{1}{2}$ |
| 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 $a$ $\bar{1}$                                   | $0, 0, 0$ $0, \frac{1}{2}, \frac{1}{2}$   |

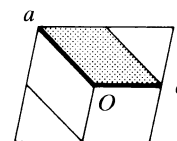
Reflection conditions

General:

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

Special: as above, plus

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

$P12_1/n1$ UNIQUE AXIS  $b$ , CELL CHOICE 2Origin at  $\bar{1}$ Asymmetric unit  $0 \leq x \leq 1$ ;  $0 \leq y \leq \frac{1}{4}$ ;  $0 \leq z \leq 1$ Generators selected (1);  $t(1,0,0)$ ;  $t(0,1,0)$ ;  $t(0,0,1)$ ; (2); (3)

## Positions

Multiplicity,  
Wyckoff letter,  
Site symmetry

Coordinates

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

Reflection conditions

General:

$h0l : h + l = 2n$

$0k0 : k = 2n$

$h00 : h = 2n$

$00l : l = 2n$

Special: as above, plus

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

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

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

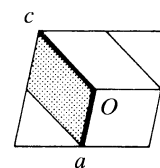
$hkl : h + k + l = 2n$

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

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

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

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

 $P12_1/a1$ UNIQUE AXIS  $b$ , CELL CHOICE 3Origin at  $\bar{1}$ Asymmetric unit  $0 \leq x \leq 1$ ;  $0 \leq y \leq \frac{1}{4}$ ;  $0 \leq z \leq 1$ Generators selected (1);  $t(1,0,0)$ ;  $t(0,1,0)$ ;  $t(0,0,1)$ ; (2); (3)

## Positions

Multiplicity,  
Wyckoff letter,  
Site symmetry

Coordinates

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

Reflection conditions

General:

$h0l : h = 2n$

$0k0 : k = 2n$

$h00 : h = 2n$

Special: as above, plus

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

$hkl : h + k = 2n$

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

$hkl : h + k = 2n$

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

$hkl : h + k = 2n$

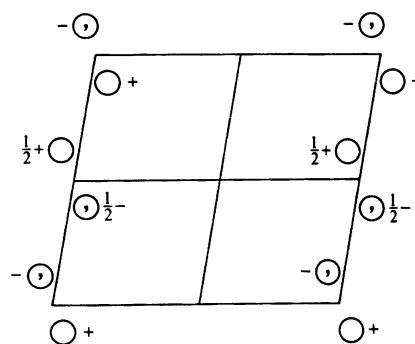
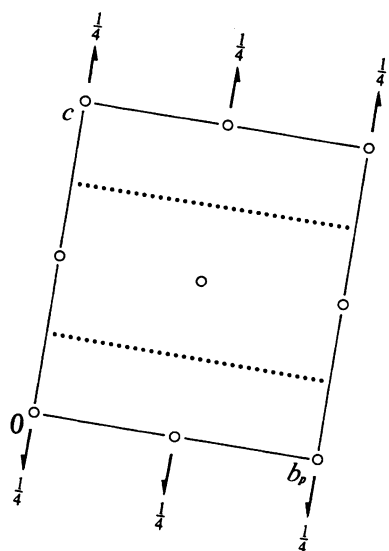
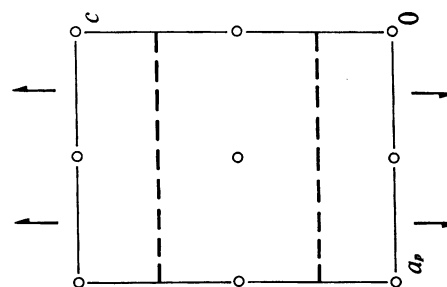
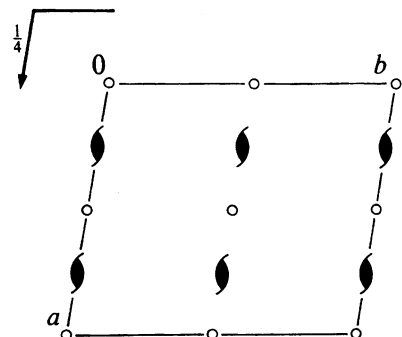
|   |     |           |           |                               |
|---|-----|-----------|-----------|-------------------------------|
| 2 | $a$ | $\bar{1}$ | $0, 0, 0$ | $\frac{1}{2}, \frac{1}{2}, 0$ |
|---|-----|-----------|-----------|-------------------------------|

$hkl : h + k = 2n$

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

Monoclinic

No. 14

 $P112_1/a$ Patterson symmetry  $P112/m$ UNIQUE AXIS  $c$ , CELL CHOICE 1Origin at  $\bar{1}$ Asymmetric unit  $0 \leq x \leq 1; 0 \leq y \leq 1; 0 \leq z \leq \frac{1}{4}$ 

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,<br>Wyckoff letter,<br>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) $x + \frac{1}{2}, y, \bar{z} + \frac{1}{2}$ | $hk0 : h = 2n$<br>$00l : l = 2n$<br>$h00 : h = 2n$ |
|   |                               |   |                                 |   | 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**

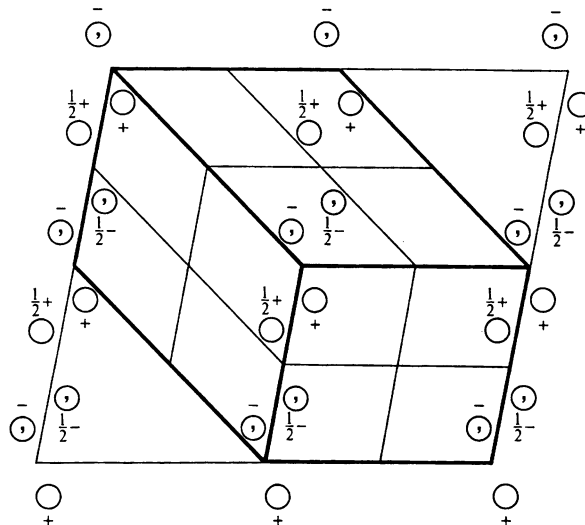
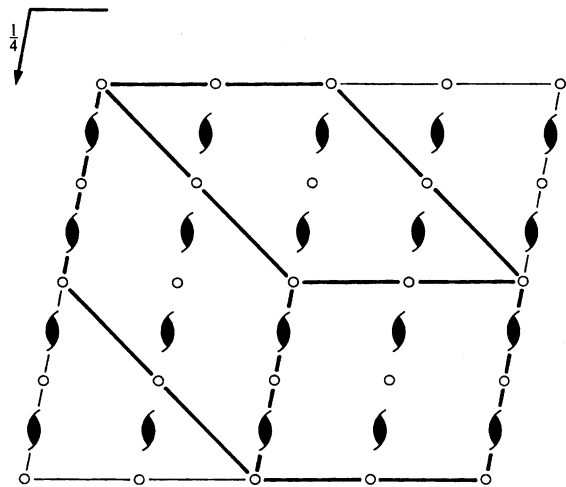
**I**     $[2] Pnna (52)$ ;  $[2] Pmna (53)$ ;  $[2] Pcca (54)$ ;  $[2] Pbam (55)$ ;  $[2] Pccn (56)$ ;  $[2] Pbcm (57)$ ;  $[2] Pnnm (58)$ ;  $[2] Pbcn (60)$ ;  
       $[2] Pbca (61)$ ;  $[2] Pnma (62)$ ;  $[2] Cmce (64)$

**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

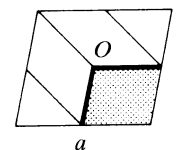
UNIQUE AXIS  $c$ , DIFFERENT CELL CHOICES $P112_1/a$ UNIQUE AXIS  $c$ , CELL CHOICE 1Origin at  $\bar{1}$ Asymmetric unit  $0 \leq x \leq 1; 0 \leq y \leq 1; 0 \leq z \leq \frac{1}{4}$ Generators selected (1);  $t(1,0,0)$ ;  $t(0,1,0)$ ;  $t(0,0,1)$ ; (2); (3)

Positions

Multiplicity,  
Wyckoff letter,  
Site symmetry

Coordinates

| Multiplicity,<br>Wyckoff letter,<br>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 $a$ $\bar{1}$                                   | $0, 0, 0$ $\frac{1}{2}, 0, \frac{1}{2}$   |



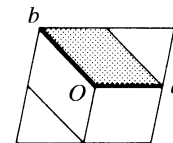
Reflection conditions

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) $x + \frac{1}{2}, y + \frac{1}{2}, \bar{z} + \frac{1}{2}$ |
|---|-----|---|---------------|---|---------------------------------|---|

Reflection conditions

General:

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

Special: as above, plus

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

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

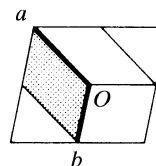
|   |     |           |                               |                     |
|---|-----|-----------|-------------------------------|---------------------|
| 2 | $c$ | $\bar{1}$ | $\frac{1}{2}, \frac{1}{2}, 0$ | $0, 0, \frac{1}{2}$ |
|---|-----|-----------|-------------------------------|---------------------|

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

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

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

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

 $hkl : h + k + l = 2n$  $P112_1/b$ 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) $x, y + \frac{1}{2}, \bar{z} + \frac{1}{2}$ |
|---|-----|---|---------------|---|---------------------------------|---|

Reflection conditions

General:

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

Special: as above, plus

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

 $hkl : k + l = 2n$ 

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

 $hkl : k + l = 2n$ 

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

 $hkl : k + l = 2n$ 

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

 $hkl : k + l = 2n$