

$Pn\bar{1}n$

$D_{2h}^2$

$mmm$

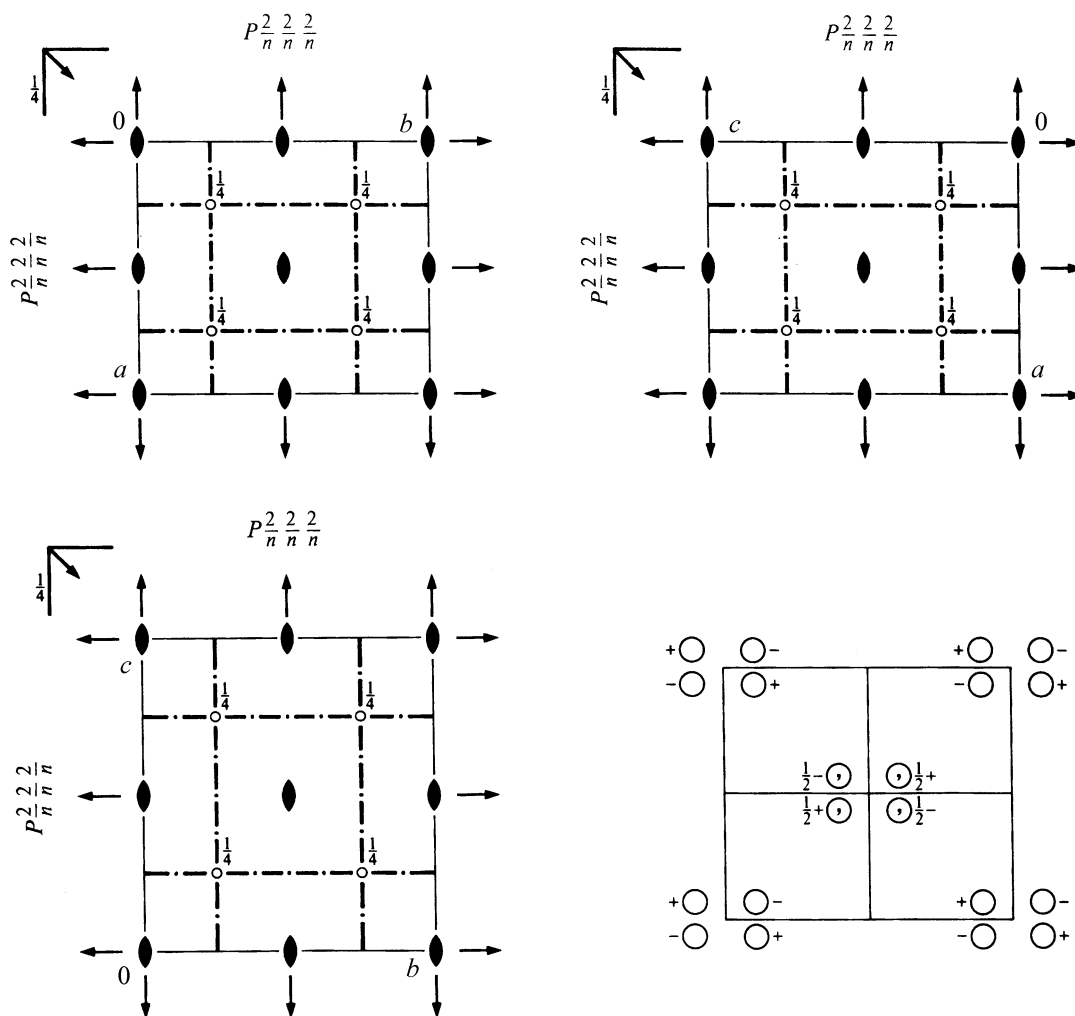
Orthorhombic

No. 48

$P 2/n 2/n 2/n$

Patterson symmetry  $Pmmm$

ORIGIN CHOICE 1



Origin at  $222$ , at  $\frac{1}{4}, \frac{1}{4}, \frac{1}{4}$  from  $\bar{1}$

Asymmetric unit  $0 \leq x \leq \frac{1}{4}; 0 \leq y \leq \frac{1}{2}; 0 \leq z \leq 1$

Symmetry operations

- |   |  |  |  |
|---|--|--|--|
| (1) 1   | (2) $2 \ 0, 0, z$  | (3) $2 \ 0, y, 0$  | (4) $2 \ x, 0, 0$  |
| (5) $\bar{1} \ \frac{1}{4}, \frac{1}{4}, \frac{1}{4}$ | (6) $n(\frac{1}{2}, \frac{1}{2}, 0) \ x, y, \frac{1}{4}$ | (7) $n(\frac{1}{2}, 0, \frac{1}{2}) \ x, \frac{1}{4}, z$ | (8) $n(0, \frac{1}{2}, \frac{1}{2}) \ \frac{1}{4}, y, z$ |

**Generators selected** (1);  $t(1,0,0)$ ;  $t(0,1,0)$ ;  $t(0,0,1)$ ; (2); (3); (5)

**Positions**

Multiplicity, Wyckoff letter, Site symmetry		Coordinates				Reflection conditions
<b>General:</b>						
8	<i>m</i> 1	(1) $x, y, z$ (5) $\bar{x} + \frac{1}{2}, \bar{y} + \frac{1}{2}, \bar{z} + \frac{1}{2}$	(2) $\bar{x}, \bar{y}, z$ (6) $x + \frac{1}{2}, y + \frac{1}{2}, \bar{z} + \frac{1}{2}$	(3) $\bar{x}, y, \bar{z}$ (7) $x + \frac{1}{2}, \bar{y} + \frac{1}{2}, z + \frac{1}{2}$	(4) $x, \bar{y}, \bar{z}$ (8) $\bar{x} + \frac{1}{2}, y + \frac{1}{2}, z + \frac{1}{2}$	$Ok\bar{l}: k + l = 2n$ $h0l: h + l = 2n$ $hk0: h + k = 2n$ $h00: h = 2n$ $0k0: k = 2n$ $00l: l = 2n$
<b>Special: as above, plus</b>						
4	<i>l</i> ..2	$0, \frac{1}{2}, z$	$0, \frac{1}{2}, \bar{z}$	$\frac{1}{2}, 0, \bar{z} + \frac{1}{2}$	$\frac{1}{2}, 0, z + \frac{1}{2}$	$hkl: h + k + l = 2n$
4	<i>k</i> ..2	$0, 0, z$	$0, 0, \bar{z}$	$\frac{1}{2}, \frac{1}{2}, \bar{z} + \frac{1}{2}$	$\frac{1}{2}, \frac{1}{2}, z + \frac{1}{2}$	$hkl: h + k + l = 2n$
4	<i>j</i> .2.	$\frac{1}{2}, y, 0$	$\frac{1}{2}, \bar{y}, 0$	$0, \bar{y} + \frac{1}{2}, \frac{1}{2}$	$0, y + \frac{1}{2}, \frac{1}{2}$	$hkl: h + k + l = 2n$
4	<i>i</i> .2.	$0, y, 0$	$0, \bar{y}, 0$	$\frac{1}{2}, \bar{y} + \frac{1}{2}, \frac{1}{2}$	$\frac{1}{2}, y + \frac{1}{2}, \frac{1}{2}$	$hkl: h + k + l = 2n$
4	<i>h</i> 2..	$x, 0, \frac{1}{2}$	$\bar{x}, 0, \frac{1}{2}$	$\bar{x} + \frac{1}{2}, \frac{1}{2}, 0$	$x + \frac{1}{2}, \frac{1}{2}, 0$	$hkl: h + k + l = 2n$
4	<i>g</i> 2..	$x, 0, 0$	$\bar{x}, 0, 0$	$\bar{x} + \frac{1}{2}, \frac{1}{2}, \frac{1}{2}$	$x + \frac{1}{2}, \frac{1}{2}, \frac{1}{2}$	$hkl: h + k + l = 2n$
4	<i>f</i> $\bar{1}$	$\frac{3}{4}, \frac{3}{4}, \frac{3}{4}$	$\frac{1}{4}, \frac{1}{4}, \frac{3}{4}$	$\frac{1}{4}, \frac{3}{4}, \frac{1}{4}$	$\frac{3}{4}, \frac{1}{4}, \frac{1}{4}$	$hkl: h + k, h + l, k + l = 2n$
4	<i>e</i> $\bar{1}$	$\frac{1}{4}, \frac{1}{4}, \frac{1}{4}$	$\frac{3}{4}, \frac{3}{4}, \frac{1}{4}$	$\frac{3}{4}, \frac{1}{4}, \frac{3}{4}$	$\frac{1}{4}, \frac{3}{4}, \frac{3}{4}$	$hkl: h + k, h + l, k + l = 2n$
2	<i>d</i> 222	$0, \frac{1}{2}, 0$	$\frac{1}{2}, 0, \frac{1}{2}$			$hkl: h + k + l = 2n$
2	<i>c</i> 222	$0, 0, \frac{1}{2}$	$\frac{1}{2}, \frac{1}{2}, 0$			$hkl: h + k + l = 2n$
2	<i>b</i> 222	$\frac{1}{2}, 0, 0$	$0, \frac{1}{2}, \frac{1}{2}$			$hkl: h + k + l = 2n$
2	<i>a</i> 222	$0, 0, 0$	$\frac{1}{2}, \frac{1}{2}, \frac{1}{2}$			$hkl: h + k + l = 2n$

**Symmetry of special projections**

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

Along [100]  $c2mm$   
 $\mathbf{a}' = \mathbf{b}$      $\mathbf{b}' = \mathbf{c}$   
 Origin at  $x, 0, 0$

Along [010]  $c2mm$   
 $\mathbf{a}' = \mathbf{c}$      $\mathbf{b}' = \mathbf{a}$   
 Origin at  $0, y, 0$

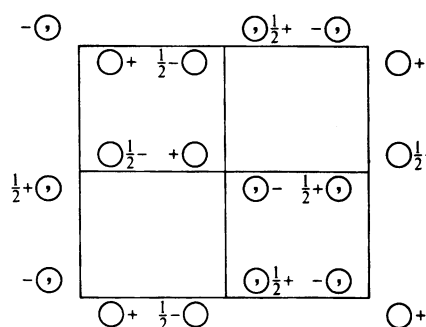
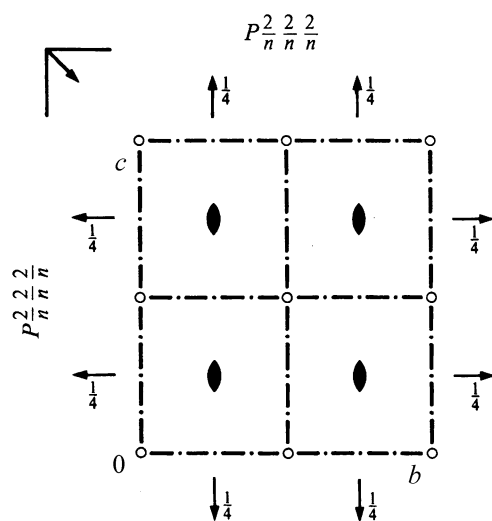
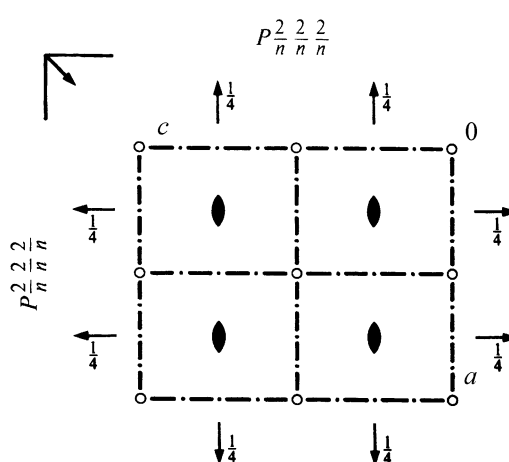
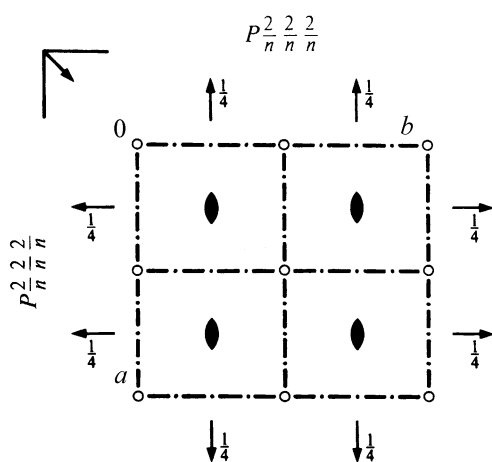
$Pnnn$  $D_{2h}^2$  $mmm$ 

Orthorhombic

No. 48

 $P 2/n 2/n 2/n$ Patterson symmetry  $Pmmm$ 

ORIGIN CHOICE 2

Origin at  $\bar{1}$  at  $nnn$ , at  $-\frac{1}{4}, -\frac{1}{4}, -\frac{1}{4}$  from 222Asymmetric unit  $0 \leq x \leq \frac{1}{4}$ ;  $-\frac{1}{4} \leq y \leq \frac{1}{4}$ ;  $0 \leq z \leq 1$ 

Symmetry operations

- |                     |  |  |  |
|---------------------|--|--|--|
| (1) 1               | (2) 2 $\frac{1}{4}, \frac{1}{4}, z$            | (3) 2 $\frac{1}{4}, y, \frac{1}{4}$            | (4) 2 $x, \frac{1}{4}, \frac{1}{4}$            |
| (5) $\bar{1}$ 0,0,0 | (6) $n(\frac{1}{2}, \frac{1}{2}, 0)$ $x, y, 0$ | (7) $n(\frac{1}{2}, 0, \frac{1}{2})$ $x, 0, z$ | (8) $n(0, \frac{1}{2}, \frac{1}{2})$ $0, y, z$ |

**Generators selected** (1);  $t(1,0,0)$ ;  $t(0,1,0)$ ;  $t(0,0,1)$ ; (2); (3); (5)

**Positions**

Multiplicity, Wyckoff letter, Site symmetry		Coordinates				Reflection conditions
<b>General:</b>						
8	<i>m</i> 1	(1) $x, y, z$ (5) $\bar{x}, \bar{y}, \bar{z}$	(2) $\bar{x} + \frac{1}{2}, \bar{y} + \frac{1}{2}, z$ (6) $x + \frac{1}{2}, y + \frac{1}{2}, \bar{z}$	(3) $\bar{x} + \frac{1}{2}, y, \bar{z} + \frac{1}{2}$ (7) $x + \frac{1}{2}, \bar{y}, z + \frac{1}{2}$	(4) $x, \bar{y} + \frac{1}{2}, \bar{z} + \frac{1}{2}$ (8) $\bar{x}, y + \frac{1}{2}, z + \frac{1}{2}$	$Ok\bar{l}: k + l = 2n$ $h0\bar{l}: h + l = 2n$ $hk0: h + k = 2n$ $h00: h = 2n$ $0k0: k = 2n$ $00\bar{l}: l = 2n$
<b>Special: as above, plus</b>						
4	<i>l</i> .. 2	$\frac{1}{4}, \frac{3}{4}, z$	$\frac{1}{4}, \frac{3}{4}, \bar{z} + \frac{1}{2}$	$\frac{3}{4}, \frac{1}{4}, \bar{z}$	$\frac{3}{4}, \frac{1}{4}, z + \frac{1}{2}$	$hkl: h + k + l = 2n$
4	<i>k</i> .. 2	$\frac{1}{4}, \frac{1}{4}, z$	$\frac{1}{4}, \frac{1}{4}, \bar{z} + \frac{1}{2}$	$\frac{3}{4}, \frac{3}{4}, \bar{z}$	$\frac{3}{4}, \frac{3}{4}, z + \frac{1}{2}$	$hkl: h + k + l = 2n$
4	<i>j</i> . 2 .	$\frac{3}{4}, y, \frac{1}{4}$	$\frac{3}{4}, \bar{y} + \frac{1}{2}, \frac{1}{4}$	$\frac{1}{4}, \bar{y}, \frac{3}{4}$	$\frac{1}{4}, y + \frac{1}{2}, \frac{3}{4}$	$hkl: h + k + l = 2n$
4	<i>i</i> . 2 .	$\frac{1}{4}, y, \frac{1}{4}$	$\frac{1}{4}, \bar{y} + \frac{1}{2}, \frac{1}{4}$	$\frac{3}{4}, \bar{y}, \frac{3}{4}$	$\frac{3}{4}, y + \frac{1}{2}, \frac{3}{4}$	$hkl: h + k + l = 2n$
4	<i>h</i> 2 ..	$x, \frac{1}{4}, \frac{3}{4}$	$\bar{x} + \frac{1}{2}, \frac{1}{4}, \frac{3}{4}$	$\bar{x}, \frac{3}{4}, \frac{1}{4}$	$x + \frac{1}{2}, \frac{3}{4}, \frac{1}{4}$	$hkl: h + k + l = 2n$
4	<i>g</i> 2 ..	$x, \frac{1}{4}, \frac{1}{4}$	$\bar{x} + \frac{1}{2}, \frac{1}{4}, \frac{1}{4}$	$\bar{x}, \frac{3}{4}, \frac{3}{4}$	$x + \frac{1}{2}, \frac{3}{4}, \frac{3}{4}$	$hkl: h + k + l = 2n$
4	<i>f</i> $\bar{1}$	0, 0, 0	$\frac{1}{2}, \frac{1}{2}, 0$	$\frac{1}{2}, 0, \frac{1}{2}$	$0, \frac{1}{2}, \frac{1}{2}$	$hkl: h + k, h + l, k + l = 2n$
4	<i>e</i> $\bar{1}$	$\frac{1}{2}, \frac{1}{2}, \frac{1}{2}$	$0, 0, \frac{1}{2}$	$0, \frac{1}{2}, 0$	$\frac{1}{2}, 0, 0$	$hkl: h + k, h + l, k + l = 2n$
2	<i>d</i> 2 2 2	$\frac{1}{4}, \frac{3}{4}, \frac{1}{4}$	$\frac{3}{4}, \frac{1}{4}, \frac{3}{4}$			$hkl: h + k + l = 2n$
2	<i>c</i> 2 2 2	$\frac{1}{4}, \frac{1}{4}, \frac{3}{4}$	$\frac{3}{4}, \frac{3}{4}, \frac{1}{4}$			$hkl: h + k + l = 2n$
2	<i>b</i> 2 2 2	$\frac{3}{4}, \frac{1}{4}, \frac{1}{4}$	$\frac{1}{4}, \frac{3}{4}, \frac{3}{4}$			$hkl: h + k + l = 2n$
2	<i>a</i> 2 2 2	$\frac{1}{4}, \frac{1}{4}, \frac{1}{4}$	$\frac{3}{4}, \frac{3}{4}, \frac{3}{4}$			$hkl: h + k + l = 2n$

**Symmetry of special projections**

Along [001]  $c2mm$

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

Origin at  $\frac{1}{4}, \frac{1}{4}, z$

Along [100]  $c2mm$

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

Origin at  $x, \frac{1}{4}, \frac{1}{4}$

Along [010]  $c2mm$

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

Origin at  $\frac{1}{4}, y, \frac{1}{4}$