

$Pn\bar{1}n$

$D_{2h}^2$

$mmm$

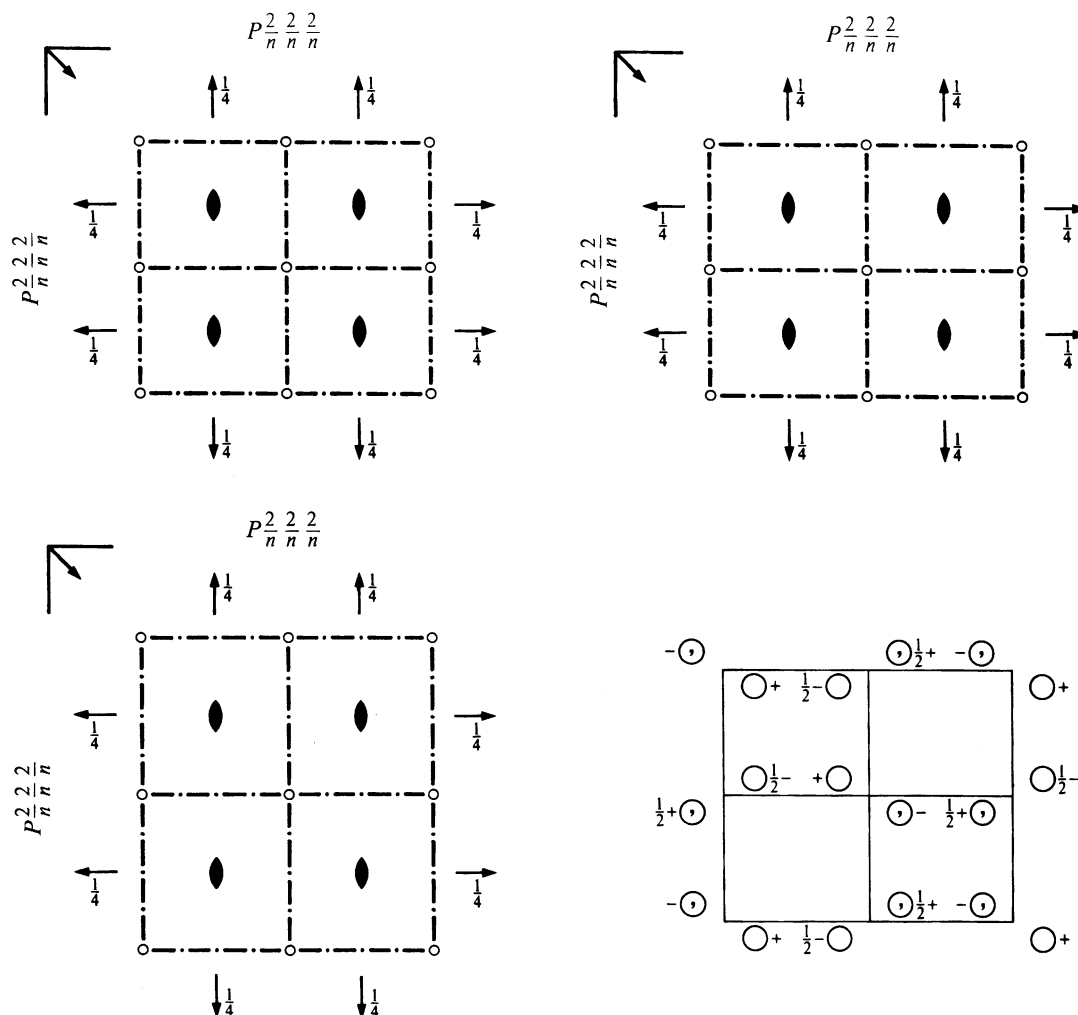
Orthorhombic

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 222

Asymmetric 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) $n(0, \frac{1}{2}, \frac{1}{2})$ $0, y, z$ |

Maximal isomorphic subgroups of lowest index

**Ic** [3]  $Pn\bar{1}n$  ( $\mathbf{a}' = 3\mathbf{a}$  or  $\mathbf{b}' = 3\mathbf{b}$  or  $\mathbf{c}' = 3\mathbf{c}$ ) (48)

Minimal non-isomorphic supergroups

**I** [2]  $P4/nnc$  (126); [2]  $P4_2/nm$  (134); [3]  $Pn\bar{3}$  (201)

**II** [2]  $Immm$  (71); [2]  $Amaa$  ( $Cccm$ , 66); [2]  $Bbmb$  ( $Cccm$ , 66); [2]  $Cccm$  (66); [2]  $Pncb$  ( $\mathbf{a}' = \frac{1}{2}\mathbf{a}$ ) ( $Pban$ , 50); [2]  $Pcna$  ( $\mathbf{b}' = \frac{1}{2}\mathbf{b}$ ) ( $Pban$ , 50); [2]  $Pban$  ( $\mathbf{c}' = \frac{1}{2}\mathbf{c}$ ) (50)

**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
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) $\bar{x}, y + \frac{1}{2}, z + \frac{1}{2}$	<b>General:</b> $Ok\bar{l} : k + l = 2n$ $h0l : h + l = 2n$ $hk0 : h + k = 2n$ $h00 : h = 2n$ $0k0 : k = 2n$ $00l : l = 2n$  <b>Special: as above, plus</b> $hkl : h + k + l = 2n$
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> 222	$\frac{1}{4}, \frac{3}{4}, \frac{1}{4}$	$\frac{3}{4}, \frac{1}{4}, \frac{3}{4}$			$hkl : h + k + l = 2n$
2 <i>c</i> 222	$\frac{1}{4}, \frac{1}{4}, \frac{3}{4}$	$\frac{3}{4}, \frac{3}{4}, \frac{1}{4}$			$hkl : h + k + l = 2n$
2 <i>b</i> 222	$\frac{3}{4}, \frac{1}{4}, \frac{1}{4}$	$\frac{1}{4}, \frac{3}{4}, \frac{3}{4}$			$hkl : h + k + l = 2n$
2 <i>a</i> 222	$\frac{1}{4}, \frac{1}{4}, \frac{1}{4}$	$\frac{3}{4}, \frac{3}{4}, \frac{3}{4}$			$hkl : h + k + l = 2n$

**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  $\frac{1}{4}, y, \frac{1}{4}$

**Maximal non-isomorphic subgroups**

<b>I</b>	[2] $Pnn2$ (34)	1; 2; 7; 8
	[2] $Pn2n$ ( $Pnn2$ , 34)	1; 3; 6; 8
	[2] $P2nn$ ( $Pnn2$ , 34)	1; 4; 6; 7
	[2] $P222$ (16)	1; 2; 3; 4
	[2] $P112/n$ ( $P2/c$ , 13)	1; 2; 5; 6
	[2] $P12/n1$ ( $P2/c$ , 13)	1; 3; 5; 7
	[2] $P2/n11$ ( $P2/c$ , 13)	1; 4; 5; 8

**IIa** none

**IIb** [2]  $Fddd$  ( $\mathbf{a}' = 2\mathbf{a}, \mathbf{b}' = 2\mathbf{b}, \mathbf{c}' = 2\mathbf{c}$ ) (70)

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