

*Pban*

$D_{2h}^4$

*mmm*

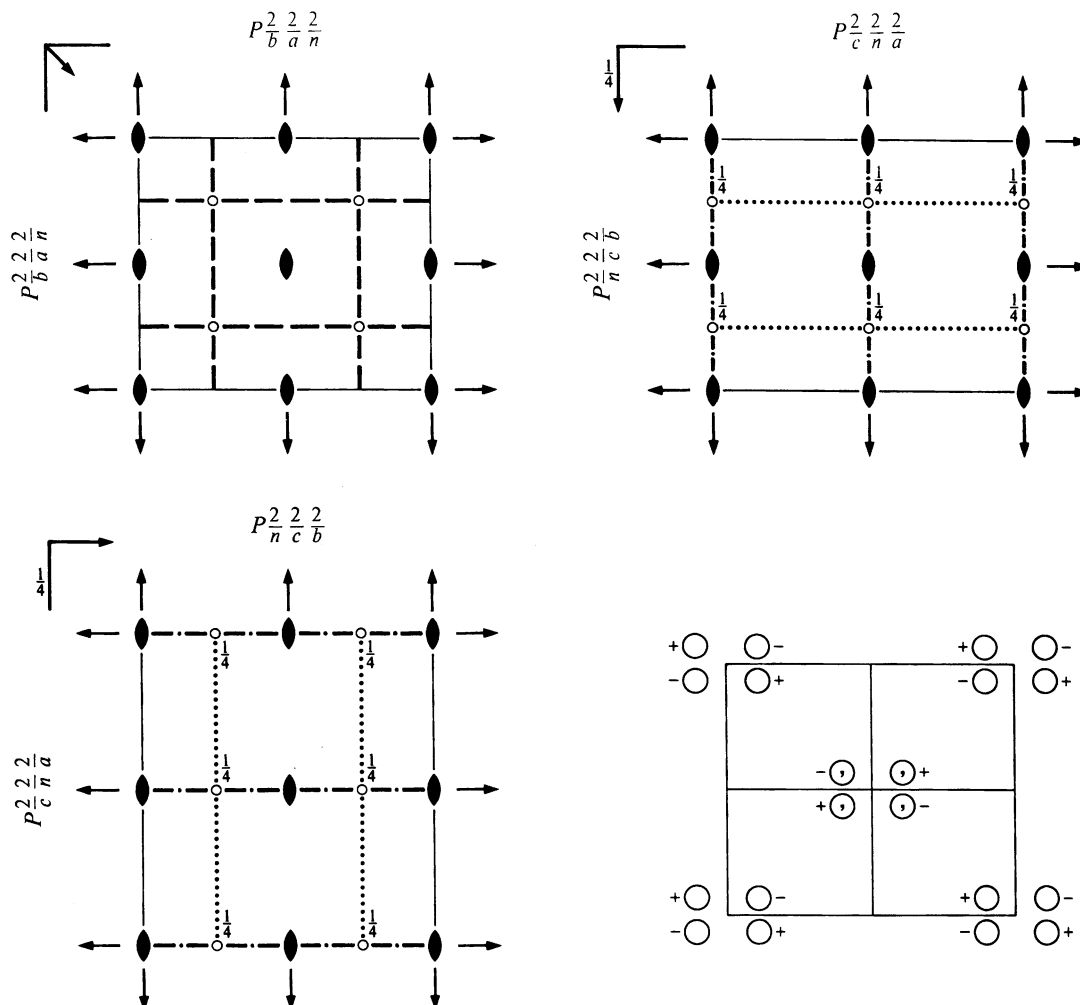
Orthorhombic

No. 50

$P\ 2/b\ 2/a\ 2/n$

Patterson symmetry  $Pmmm$

ORIGIN CHOICE 1



Origin at  $222/n$ , at  $\frac{1}{4}, \frac{1}{4}, 0$  from  $\bar{1}$

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

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

**Minimal non-isomorphic supergroups**

**I** [2]  $P4/nbm$  (125); [2]  $P4_2/nbc$  (133)

**II** [2]  $Cmmm$  (65); [2]  $Aeaa$  ( $Ccce$ , 68); [2]  $Bbeb$  ( $Ccce$ , 68); [2]  $Ibam$  (72); [2]  $Pbmb$  ( $\mathbf{a}' = \frac{1}{2}\mathbf{a}$ ) ( $Pccm$ , 49); [2]  $Pmaa$  ( $\mathbf{b}' = \frac{1}{2}\mathbf{b}$ ) ( $Pccm$ , 49)

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

**Symmetry of special projections**

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

Along [100]  $p2mm$   
 $\mathbf{a}' = \frac{1}{2}\mathbf{b}$      $\mathbf{b}' = \mathbf{c}$   
 Origin at x, 0, 0

Along [010]  $p2mm$   
 $\mathbf{a}' = \mathbf{c}$      $\mathbf{b}' = \frac{1}{2}\mathbf{a}$   
 Origin at 0, y, 0

**Maximal non-isomorphic subgroups**

<b>I</b>	[2] <i>Pba2</i> (32)	1; 2; 7; 8
	[2] <i>Pb2n</i> ( <i>Pnc</i> 2, 30)	1; 3; 6; 8
	[2] <i>P2an</i> ( <i>Pnc</i> 2, 30)	1; 4; 6; 7
	[2] <i>P222</i> (16)	1; 2; 3; 4
	[2] <i>P112/n</i> ( <i>P2/c</i> , 13)	1; 2; 5; 6
	[2] <i>P12/a1</i> ( <i>P2/c</i> , 13)	1; 3; 5; 7
[2] <i>P2/b11</i> ( <i>P2/c</i> , 13)	1; 4; 5; 8	

**IIa** none

**IIb** [2] *Pnan* ( $\mathbf{c}' = 2\mathbf{c}$ ) (*Pnna*, 52); [2] *Pbnn* ( $\mathbf{c}' = 2\mathbf{c}$ ) (*Pnna*, 52); [2] *Pnnn* ( $\mathbf{c}' = 2\mathbf{c}$ ) (48)

**Maximal isomorphic subgroups of lowest index**

**IIc** [2] *Pban* ( $\mathbf{c}' = 2\mathbf{c}$ ) (50); [3] *Pban* ( $\mathbf{a}' = 3\mathbf{a}$  or  $\mathbf{b}' = 3\mathbf{b}$ ) (50)

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