

$Pbcn$

$D_{2h}^{14}$

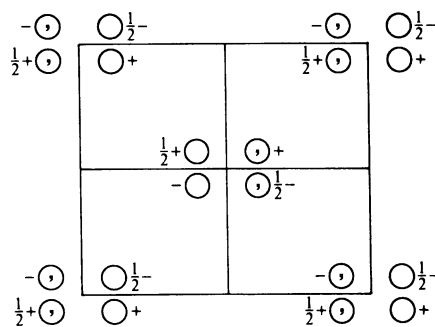
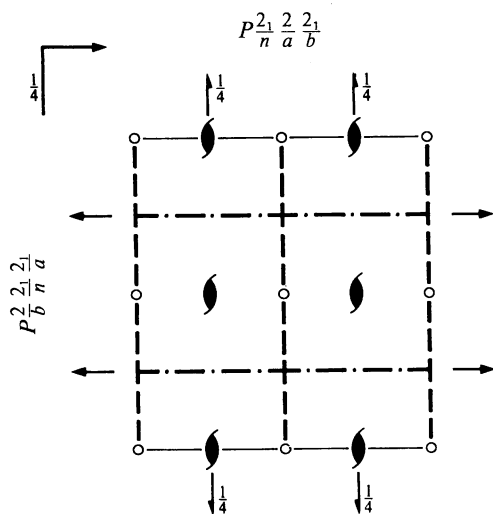
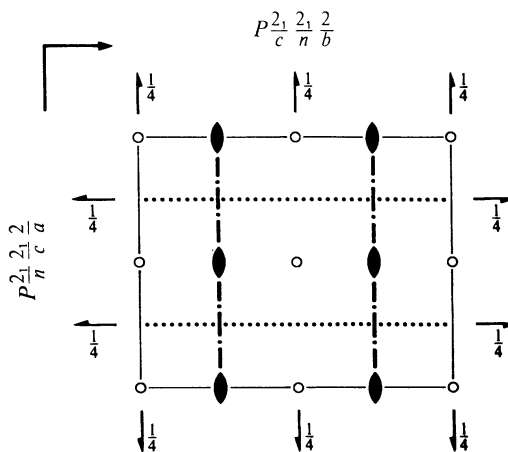
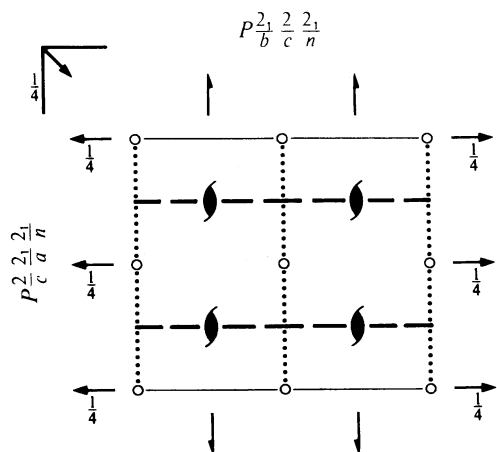
$mmm$

Orthorhombic

No. 60

$P 2_1/b 2/c 2_1/n$

Patterson symmetry  $Pmmm$



Origin at  $\bar{1}$  on  $1c1$

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

**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>d</i> 1	(1) $x, y, z$	(2) $\bar{x} + \frac{1}{2}, \bar{y} + \frac{1}{2}, z + \frac{1}{2}$	(3) $\bar{x}, y, \bar{z} + \frac{1}{2}$	(4) $x + \frac{1}{2}, \bar{y} + \frac{1}{2}, \bar{z}$	$Ok\bar{l} : k = 2n$
	(5) $\bar{x}, \bar{y}, \bar{z}$	(6) $x + \frac{1}{2}, y + \frac{1}{2}, \bar{z} + \frac{1}{2}$	(7) $x, \bar{y}, z + \frac{1}{2}$	(8) $\bar{x} + \frac{1}{2}, y + \frac{1}{2}, z$	$h0\bar{l} : l = 2n$
					$hk0 : h + k = 2n$
					$h00 : h = 2n$
					$0k0 : k = 2n$
					$00\bar{l} : l = 2n$
					<b>Special: as above, plus</b>
4 <i>c</i> .2.	$0, y, \frac{1}{4}$	$\frac{1}{2}, \bar{y} + \frac{1}{2}, \frac{3}{4}$	$0, \bar{y}, \frac{3}{4}$	$\frac{1}{2}, y + \frac{1}{2}, \frac{1}{4}$	$hkl : h + k = 2n$
4 <i>b</i> $\bar{1}$	$0, \frac{1}{2}, 0$	$\frac{1}{2}, 0, \frac{1}{2}$	$0, \frac{1}{2}, \frac{1}{2}$	$\frac{1}{2}, 0, 0$	$hkl : h + k, l = 2n$
4 <i>a</i> $\bar{1}$	$0, 0, 0$	$\frac{1}{2}, \frac{1}{2}, \frac{1}{2}$	$0, 0, \frac{1}{2}$	$\frac{1}{2}, \frac{1}{2}, 0$	$hkl : h + k, l = 2n$

**Symmetry of special projections**

Along [001]  $c2mm$

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

Origin at 0, 0, z

Along [100]  $p2gm$

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

Origin at x, 0, 0

Along [010]  $p2gm$

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

Origin at 0, y, 0

**Maximal non-isomorphic subgroups**

<b>I</b>	[2] $P2_1cn$ ( $Pna2_1$ , 33)	1; 4; 6; 7
	[2] $Pb2n$ ( $Pnc2$ , 30)	1; 3; 6; 8
	[2] $Pbc2_1$ ( $Pca2_1$ , 29)	1; 2; 7; 8
	[2] $P2_12_2$ ( $P2_12_1$ , 18)	1; 2; 3; 4
	[2] $P112_1/n$ ( $P2_1/c$ , 14)	1; 2; 5; 6
	[2] $P2_1/b11$ ( $P2_1/c$ , 14)	1; 4; 5; 8
	[2] $P12/c1$ ( $P2/c$ , 13)	1; 3; 5; 7

**IIa** none

**IIb** none

**Maximal isomorphic subgroups of lowest index**

**IIc** [3]  $Pbcn$  ( $\mathbf{a}' = 3\mathbf{a}$ ) (60); [3]  $Pbcn$  ( $\mathbf{b}' = 3\mathbf{b}$ ) (60); [3]  $Pbcn$  ( $\mathbf{c}' = 3\mathbf{c}$ ) (60)

**Minimal non-isomorphic supergroups**

**I** none

**II** [2]  $Cmcm$  (63); [2]  $Aema$  ( $Cmce$ , 64); [2]  $Bbeb$  ( $Ccce$ , 68); [2]  $Ibam$  (72); [2]  $Pbmn$  ( $\mathbf{c}' = \frac{1}{2}\mathbf{c}$ ) ( $Pmna$ , 53); [2]  $Pbcb$  ( $\mathbf{a}' = \frac{1}{2}\mathbf{a}$ ) ( $Pcca$ , 54); [2]  $Pmca$  ( $\mathbf{b}' = \frac{1}{2}\mathbf{b}$ ) ( $Pbcm$ , 57)