

*Pbam*

$D_{2h}^9$

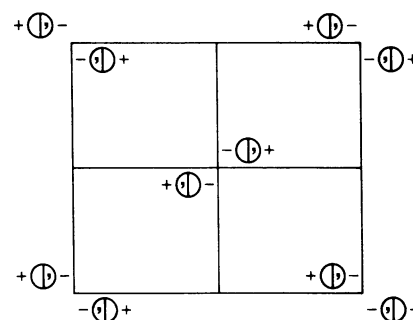
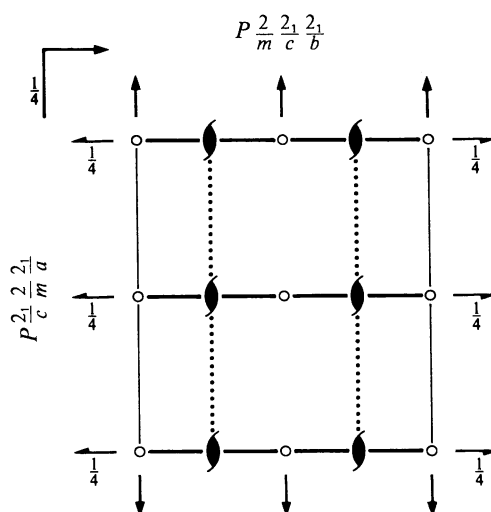
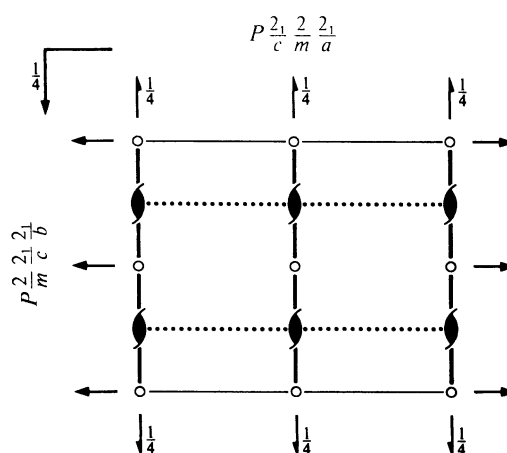
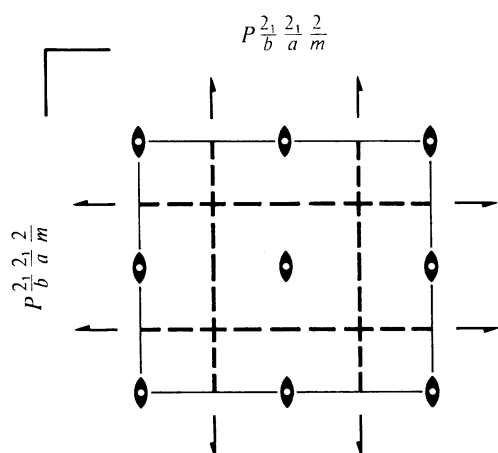
*mmm*

Orthorhombic

No. 55

$P 2_1/b 2_1/a 2/m$

Patterson symmetry *Pmmm*



Origin at centre ( $2/m$ )

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) $2(0, \frac{1}{2}, 0)$ $\frac{1}{4}, y, 0$ | (4) $2(\frac{1}{2}, 0, 0)$ $x, \frac{1}{4}, 0$ |
| (5) $\bar{1}$ $0, 0, 0$ | (6) $m$ $x, y, 0$ | (7) $a$ $x, \frac{1}{4}, z$                    | (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
8 <i>i</i> 1	(1) $x, y, z$ (5) $\bar{x}, \bar{y}, \bar{z}$	(2) $\bar{x}, \bar{y}, z$ (6) $x, y, \bar{z}$	(3) $\bar{x} + \frac{1}{2}, y + \frac{1}{2}, \bar{z}$ (7) $x + \frac{1}{2}, \bar{y} + \frac{1}{2}, z$	(4) $x + \frac{1}{2}, \bar{y} + \frac{1}{2}, \bar{z}$ (8) $\bar{x} + \frac{1}{2}, y + \frac{1}{2}, z$	General: $0kl : k = 2n$ $h0l : h = 2n$ $h00 : h = 2n$ $0k0 : k = 2n$ Special: as above, plus
4 <i>h</i> .. <i>m</i>	$x, y, \frac{1}{2}$	$\bar{x}, \bar{y}, \frac{1}{2}$	$\bar{x} + \frac{1}{2}, y + \frac{1}{2}, \frac{1}{2}$	$x + \frac{1}{2}, \bar{y} + \frac{1}{2}, \frac{1}{2}$	no extra conditions
4 <i>g</i> .. <i>m</i>	$x, y, 0$	$\bar{x}, \bar{y}, 0$	$\bar{x} + \frac{1}{2}, y + \frac{1}{2}, 0$	$x + \frac{1}{2}, \bar{y} + \frac{1}{2}, 0$	no extra conditions
4 <i>f</i> .. 2	$0, \frac{1}{2}, z$	$\frac{1}{2}, 0, \bar{z}$	$0, \frac{1}{2}, \bar{z}$	$\frac{1}{2}, 0, z$	$hkl : h + k = 2n$
4 <i>e</i> .. 2	$0, 0, z$	$\frac{1}{2}, \frac{1}{2}, \bar{z}$	$0, 0, \bar{z}$	$\frac{1}{2}, \frac{1}{2}, z$	$hkl : h + k = 2n$
2 <i>d</i> .. $2/m$	$0, \frac{1}{2}, \frac{1}{2}$	$\frac{1}{2}, 0, \frac{1}{2}$			$hkl : h + k = 2n$
2 <i>c</i> .. $2/m$	$0, \frac{1}{2}, 0$	$\frac{1}{2}, 0, 0$			$hkl : h + k = 2n$
2 <i>b</i> .. $2/m$	$0, 0, \frac{1}{2}$	$\frac{1}{2}, \frac{1}{2}, \frac{1}{2}$			$hkl : h + k = 2n$
2 <i>a</i> .. $2/m$	$0, 0, 0$	$\frac{1}{2}, \frac{1}{2}, 0$			$hkl : h + k = 2n$

**Symmetry of special projections**

Along [001]  $p2gg$   
 $\mathbf{a}' = \mathbf{a}$   $\mathbf{b}' = \mathbf{b}$   
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] $Pba2$ (32)	1; 2; 7; 8
	[2] $Pb2_1m$ ( $Pmc2_1$ , 26)	1; 3; 6; 8
	[2] $P2_1am$ ( $Pmc2_1$ , 26)	1; 4; 6; 7
	[2] $P2_12_12$ (18)	1; 2; 3; 4
	[2] $P12_1/a1$ ( $P2_1/c$ , 14)	1; 3; 5; 7
	[2] $P2_1/b11$ ( $P2_1/c$ , 14)	1; 4; 5; 8
	[2] $P112/m$ ( $P2/m$ , 10)	1; 2; 5; 6

**IIa** none

**IIb** [2]  $Pnam$  ( $\mathbf{c}' = 2\mathbf{c}$ ) ( $Pnma$ , 62); [2]  $Pbnm$  ( $\mathbf{c}' = 2\mathbf{c}$ ) ( $Pnma$ , 62); [2]  $Pnnm$  ( $\mathbf{c}' = 2\mathbf{c}$ ) (58)

**Maximal isomorphic subgroups of lowest index**

**IIc** [2]  $Pbam$  ( $\mathbf{c}' = 2\mathbf{c}$ ) (55); [3]  $Pbam$  ( $\mathbf{a}' = 3\mathbf{a}$  or  $\mathbf{b}' = 3\mathbf{b}$ ) (55)

**Minimal non-isomorphic supergroups**

**I** [2]  $P4/mbm$  (127); [2]  $P4_2/mbc$  (135)

**II** [2]  $Aeam$  ( $Cmce$ , 64); [2]  $Bbem$  ( $Cmce$ , 64); [2]  $Cmmm$  (65); [2]  $Ibam$  (72); [2]  $Pbmm$  ( $\mathbf{a}' = \frac{1}{2}\mathbf{a}$ ) ( $Pmma$ , 51); [2]  $Pmam$  ( $\mathbf{b}' = \frac{1}{2}\mathbf{b}$ ) ( $Pmma$ , 51)