

$pbam$

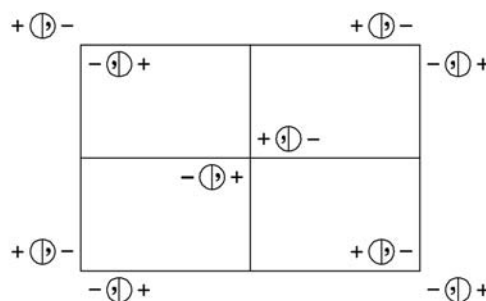
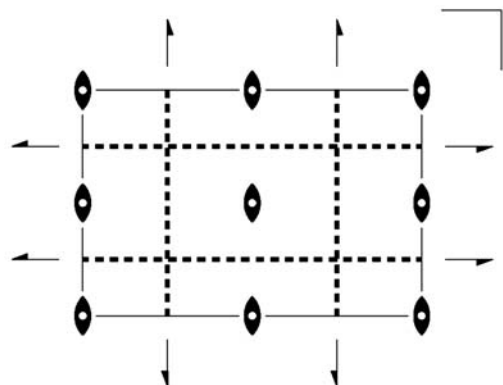
$mmm$

Orthorhombic/Rectangular

No. 44

$p2_1/b2_1/a2/m$

Patterson symmetry  $pmmm$



Origin at centre ( $2/m$ )

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

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);  $t(1,0,0)$ ;  $t(0,1,0)$ ; (2); (3); (5)

**Positions**

Multiplicity, Wyckoff letter, Site symmetry	Coordinates				Reflection conditions
8 <i>f</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: $0k: k = 2n$ $h0: h = 2n$  Special: as above, plus
4 <i>e</i> $\dots m$	$x, y, 0$	$\bar{x}, \bar{y}, 0$	$\bar{x} + \frac{1}{2}, y + \frac{1}{2}, 0$	$x + \frac{1}{2}, \bar{y} + \frac{1}{2}, 0$	no extra conditions
4 <i>d</i> $\dots 2$	$0, \frac{1}{2}, z$	$\frac{1}{2}, 0, \bar{z}$	$0, \frac{1}{2}, \bar{z}$	$\frac{1}{2}, 0, z$	$hk: h + k = 2n$
4 <i>c</i> $\dots 2$	$0, 0, z$	$\frac{1}{2}, \frac{1}{2}, \bar{z}$	$0, 0, \bar{z}$	$\frac{1}{2}, \frac{1}{2}, z$	$hk: h + k = 2n$
2 <i>b</i> $\dots 2/m$	$0, \frac{1}{2}, 0$	$\frac{1}{2}, 0, 0$			$hk: h + k = 2n$
2 <i>a</i> $\dots 2/m$	$0, 0, 0$	$\frac{1}{2}, \frac{1}{2}, 0$			$hk: h + k = 2n$

**Symmetry of special projections**

Along [001]  $p2gg$   
 $\mathbf{a}' = \mathbf{a}$      $\mathbf{b}' = \mathbf{b}$   
 Origin at  $0, 0, z$

Along [100]  $\not\neq 2mm$   
 $\mathbf{a}' = \frac{1}{2}\mathbf{b}$   
 Origin at  $x, 0, 0$

Along [010]  $\not\neq 2mm$   
 $\mathbf{a}' = \frac{1}{2}\mathbf{a}$   
 Origin at  $0, y, 0$

**Maximal non-isotypic subgroups**

<b>I</b>	[2] $pb2_1m$ (29)	1; 3; 6; 8
	[2] $p2_1am$ ( $pb2_1m, 29$ )	1; 4; 6; 7
	[2] $pba2$ (25)	1; 2; 7; 8
	[2] $p2_12_12$ (21)	1; 2; 3; 4
	[2] $p12_1/a1$ ( $p2_1/b11, 17$ )	1; 3; 5; 7
	[2] $p2_1/b11$ (17)	1; 4; 5; 8
	[2] $p112/m$ (6)	1; 2; 5; 6

**IIa** none

**IIb** none

**Maximal isotypic subgroups of lowest index**

**IIc** [3]  $pbam$  ( $\mathbf{a}' = 3\mathbf{a}$  or  $\mathbf{b}' = 3\mathbf{b}$ ) (44)

**Minimal non-isotypic supergroups**

**I** [2]  $p4/mbm$  (63)

**II** [2]  $cmmm$  (47); [2]  $pmam$  ( $\mathbf{b}' = \frac{1}{2}\mathbf{b}$ ) (40)