

$pbam$

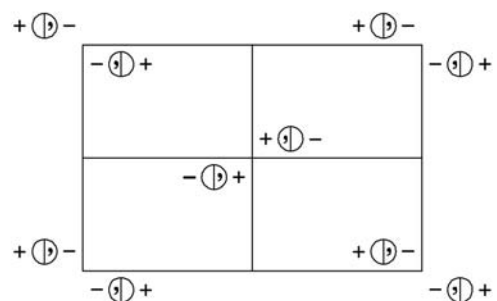
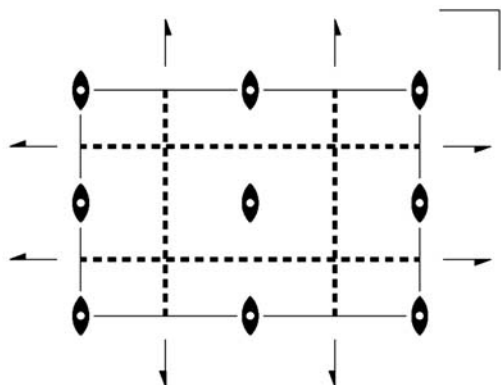
mmm

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
(1 0,0,0) | (2) 2 $0,0,z$
(2 _z 0,0,0) | (3) 2(0, $\frac{1}{2}, 0$) $\frac{1}{4}, y, 0$
(2 _y $\frac{1}{2}, \frac{1}{2}, 0$) | (4) 2($\frac{1}{2}, 0, 0$) $x, \frac{1}{4}, 0$
(2 _x $\frac{1}{2}, \frac{1}{2}, 0$) |
| (5) $\bar{1}$ 0,0,0
($\bar{1}$ 0,0,0) | (6) m $x,y,0$
(m_z 0,0,0) | (7) a $x, \frac{1}{4}, z$
(m_y $\frac{1}{2}, \frac{1}{2}, 0$) | (8) b $\frac{1}{4}, y, z$
(m_x $\frac{1}{2}, \frac{1}{2}, 0$) |

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

I	[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)