

$pbma$

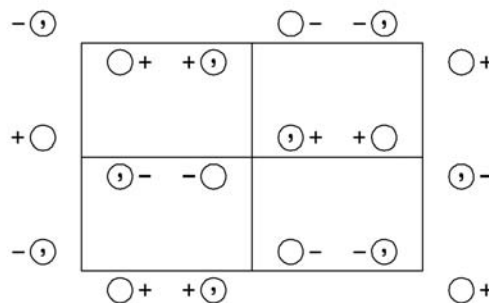
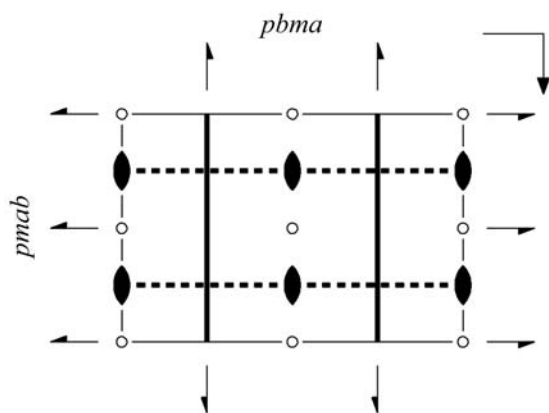
mmm

Orthorhombic/Rectangular

No. 45

$p2_1/b2_1/m2/a$

Patterson symmetry $pmmm$



Origin at $\bar{1}$ on 12_1a

Asymmetric unit $0 \leq x \leq 1; 0 \leq y \leq \frac{1}{4}; 0 \leq z$

Symmetry operations

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

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>d</i> 1	(1) x, y, z (5) $\bar{x}, \bar{y}, \bar{z}$	(2) $\bar{x}, y + \frac{1}{2}, \bar{z}$ (6) $x, \bar{y} + \frac{1}{2}, z$	(3) $x + \frac{1}{2}, \bar{y} + \frac{1}{2}, \bar{z}$ (7) $\bar{x} + \frac{1}{2}, y + \frac{1}{2}, z$	(4) $\bar{x} + \frac{1}{2}, \bar{y}, z$ (8) $x + \frac{1}{2}, y, \bar{z}$	General: $hk: h = 2n$ $h0: h = 2n$ $0k: k = 2n$ Special: as above, plus
4 <i>c</i> . <i>m</i> .	$x, \frac{1}{4}, z$	$\bar{x}, \frac{3}{4}, \bar{z}$	$x + \frac{1}{2}, \frac{1}{4}, \bar{z}$	$\bar{x} + \frac{1}{2}, \frac{3}{4}, z$	no extra conditions
4 <i>b</i> . . 2	$\frac{1}{4}, 0, z$	$\frac{3}{4}, \frac{1}{2}, \bar{z}$	$\frac{3}{4}, 0, \bar{z}$	$\frac{1}{4}, \frac{1}{2}, z$	$hk: k = 2n$
4 <i>a</i> $\bar{1}$	0, 0, 0	$0, \frac{1}{2}, 0$	$\frac{1}{2}, \frac{1}{2}, 0$	$\frac{1}{2}, 0, 0$	$hk: k = 2n$

Symmetry of special projections

Along [001] $p2mg$
 $\mathbf{a}' = \mathbf{b}$ $\mathbf{b}' = -\frac{1}{2}\mathbf{a}$
 Origin at 0, 0, z

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

Along [010] $\not{h}2mg$
 $\mathbf{a}' = \mathbf{a}$
 Origin at 0, $y, 0$

Maximal non-isotypic subgroups

I	[2] $pb2_1a$ (33)	1; 2; 7; 8
	[2] $p2_1ma$ ($pm2_1b$, 28)	1; 3; 6; 8
	[2] $pbm2$ ($pma2$, 24)	1; 4; 6; 7
	[2] $p2_12_12$ (21)	1; 2; 3; 4
	[2] $p2_1/b11$ (17)	1; 3; 5; 7
	[2] $p12_1/m1$ ($p2_1/m11$, 15)	1; 2; 5; 6
	[2] $p112/a$ (7)	1; 4; 5; 8

IIa none

IIb none

Maximal isotypic subgroups of lowest index

IIc [3] $pbma$ ($\mathbf{a}' = 3\mathbf{a}$) (45); [3] $pbma$ ($\mathbf{b}' = 3\mathbf{b}$) (45)

Minimal non-isotypic supergroups

I none

II [2] $cmme$ (48); [2] $pmam$ ($\mathbf{b}' = \frac{1}{2}\mathbf{b}$) (40); [2] $pmma$ ($\mathbf{b}' = \frac{1}{2}\mathbf{b}$) (41)