

$pb\bar{a}a$

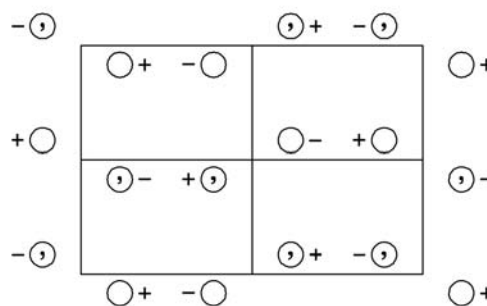
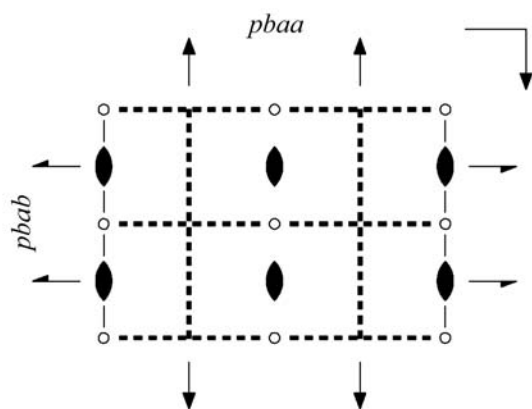
mmm

Orthorhombic/Rectangular

No. 43

$p2/b2_1/a2/a$

Patterson symmetry $pmmm$



Origin at $\bar{1}$ on $b1a$

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

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

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] $\not p2mm$
 $\mathbf{a}' = \frac{1}{2}\mathbf{b}$
Origin at $x, 0, 0$

Along [010] $\not p2mm$
 $\mathbf{a}' = \frac{1}{2}\mathbf{a}$
Origin at $0, y, 0$

Maximal non-isotypic subgroups

I	[2] $pb2, a$ (33)	1; 4; 6; 7
	[2] $p2aa$ ($pb2b, 30$)	1; 2; 7; 8
	[2] $pba2$ (25)	1; 3; 6; 8
	[2] $p22, 2$ ($p2, 22, 20$)	1; 2; 3; 4
	[2] $p12, /a1$ ($p2, /b11, 17$)	1; 4; 5; 8
	[2] $p2/b11$ (16)	1; 2; 5; 6
	[2] $p112/a$ (7)	1; 3; 5; 7

IIa none

IIb none

Maximal isotypic subgroups of lowest index

IIc [3] $pbaa$ ($\mathbf{a}' = 3\mathbf{a}$) (43); [3] $pbaa$ ($\mathbf{b}' = 3\mathbf{b}$) (43)

Minimal non-isotypic supergroups

I none

II [2] $cmme$ (48); [2] $pmaa$ ($\mathbf{b}' = \frac{1}{2}\mathbf{b}$) (38); [2] $pmam$ ($\mathbf{b}' = \frac{1}{2}\mathbf{b}$) (40)