

pban

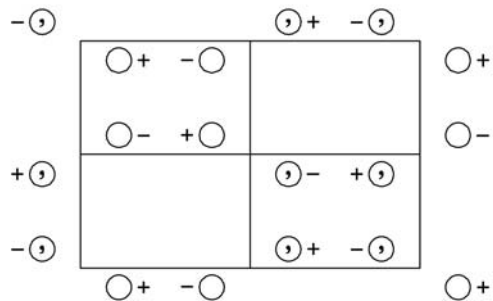
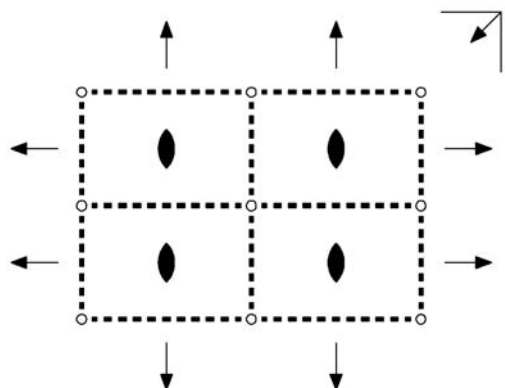
mmm

Orthorhombic/Rectangular

No. 39

p2/b2/a2/n

Patterson symmetry *pmmm*



Origin at $\bar{1}$ at *ban*, at $-\frac{1}{4}, -\frac{1}{4}, 0$ from 222

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

Symmetry operations

- | | | | |
|---------------------|--|---------------------------|---------------------------|
| (1) 1 | (2) 2 $\frac{1}{4}, \frac{1}{4}, z$ | (3) 2 $\frac{1}{4}, y, 0$ | (4) 2 $x, \frac{1}{4}, 0$ |
| (5) $\bar{1}$ 0,0,0 | (6) $n(\frac{1}{2}, \frac{1}{2}, 0)$ $x, y, 0$ | (7) a $x, 0, z$ | (8) b $0, y, z$ |

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

Symmetry of special projections

Along [001] $c2mm$

$\mathbf{a}' = \mathbf{a}$ $\mathbf{b}' = \mathbf{b}$

Origin at $\frac{1}{4}, \frac{1}{4}, z$

Along [100] $\not\sim 2mm$

$\mathbf{a}' = \frac{1}{2}\mathbf{b}$

Origin at $x, 0, 0$

Along [010] $\not\sim 2mm$

$\mathbf{a}' = \frac{1}{2}\mathbf{a}$

Origin at $0, y, 0$

Maximal non-isotypic subgroups

I	[2] $pb2n$ (34)	1; 3; 6; 8
	[2] $p2an$ ($pb2n$, 34)	1; 4; 6; 7
	[2] $pba2$ (25)	1; 2; 7; 8
	[2] $p222$ (19)	1; 2; 3; 4
	[2] $p12/a1$ ($p2/b11$, 16)	1; 3; 5; 7
	[2] $p2/b11$ (16)	1; 4; 5; 8
	[2] $p112/n$ ($p112/a$, 7)	1; 2; 5; 6

IIa none

IIb none

Maximal isotypic subgroups of lowest index

IIc [3] $pban$ ($\mathbf{a}' = 3\mathbf{a}$ or $\mathbf{b}' = 3\mathbf{b}$) (39)

Minimal non-isotypic supergroups

I [2] $p4/nbm$ (62)

II [2] $cmmm$ (47); [2] $pmaa$ ($\mathbf{b}' = \frac{1}{2}\mathbf{b}$) (38)