

pmān

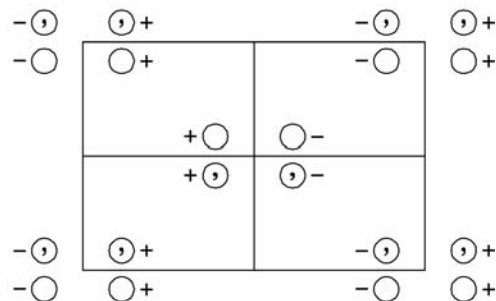
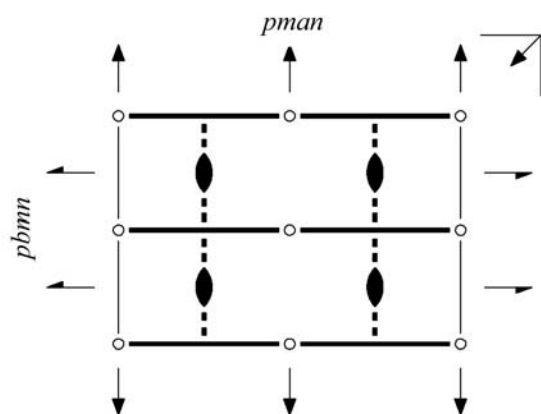
m m m

Orthorhombic/Rectangular

No. 42

p2/m2₁/a2/n

Patterson symmetry *pmmm*



Origin at centre ($2/m$) at $2/m1n$

Asymmetric unit $0 \leq x \leq \frac{1}{2}; 0 \leq y \leq \frac{1}{4}$

Symmetry operations

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

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

Symmetry of special projections

Along $[001] c2mm$
 $\mathbf{a}' = \mathbf{a}$ $\mathbf{b}' = \mathbf{b}$
Origin at $0, 0, z$

Along $[100] \not\sim 2mg$
 $\mathbf{a}' = \mathbf{b}$
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	$[2] p2an (pb2n, 34)$	1; 4; 6; 7
	$[2] pm2_1n (32)$	1; 2; 7; 8
	$[2] pma2 (24)$	1; 3; 6; 8
	$[2] p22_12 (p2_122, 20)$	1; 2; 3; 4
	$[2] p12_1/a1 (p2_1/b11, 17)$	1; 2; 5; 6
	$[2] p2/m11 (14)$	1; 4; 5; 8
	$[2] p112/n (p112/a, 7)$	1; 3; 5; 7

IIa none

IIb none

Maximal isotypic subgroups of lowest index

IIc $[3] pman (\mathbf{a}' = 3\mathbf{a}) (42)$; $[3] pman (\mathbf{b}' = 3\mathbf{b}) (42)$

Minimal non-isotypic supergroups

I none

II $[2] cmmm (47)$; $[2] pmaa (\mathbf{b}' = \frac{1}{2}\mathbf{b}) (38)$; $[2] pmma (\mathbf{b}' = \frac{1}{2}\mathbf{b}) (41)$