

$pb a 2$

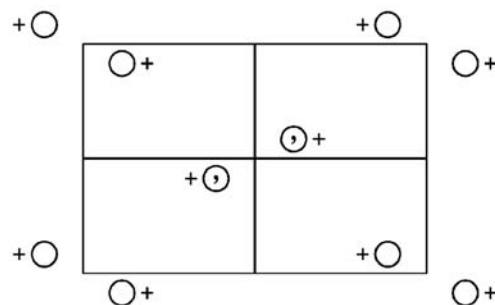
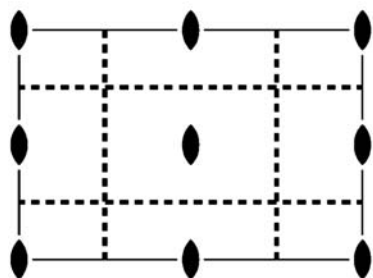
$mm 2$

Orthorhombic/Rectangular

No. 25

$pb a 2$

Patterson symmetry $pmmm$



Origin on 112

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

Symmetry operations

- (1) 1 (2) 2 $0, 0, z$ (3) a $x, \frac{1}{4}, z$ (4) b $\frac{1}{4}, y, z$

Generators selected (1); $t(1,0,0)$; $t(0,1,0)$; (2); (3)

Positions

Multiplicity, Wyckoff letter, Site symmetry	Coordinates				Reflection conditions
4 c 1	(1) x, y, z	(2) \bar{x}, \bar{y}, z	(3) $x + \frac{1}{2}, \bar{y} + \frac{1}{2}, z$	(4) $\bar{x} + \frac{1}{2}, y + \frac{1}{2}, z$	General: $h0: h = 2n$ $0k: k = 2n$ Special: as above, plus
2 b .. 2	$0, \frac{1}{2}, z$	$\frac{1}{2}, 0, z$			$hk: h + k = 2n$
2 a .. 2	$0, 0, z$	$\frac{1}{2}, \frac{1}{2}, z$			$hk: h + k = 2n$

Symmetry of special projections

Along [001] $p2gg$
 $\mathbf{a}' = \mathbf{a}$ $\mathbf{b}' = \mathbf{b}$
 Origin at $0, 0, z$

Along [100] $\cancel{1}m1$
 $\mathbf{a}' = \frac{1}{2}\mathbf{b}$
 Origin at $x, 0, 0$

Along [010] $\cancel{1}m1$
 $\mathbf{a}' = \frac{1}{2}\mathbf{a}$
 Origin at $0, y, 0$

Maximal non-isotypic subgroups

I [2] $p1a1$ ($pb11, 12$) 1; 3
 [2] $pb11$ (12) 1; 4
 [2] $p112$ (3) 1; 2

IIa none

IIb none

Maximal isotypic subgroups of lowest index

IIc [3] $pba2$ ($\mathbf{a}' = 3\mathbf{a}$ or $\mathbf{b}' = 3\mathbf{b}$) (25)

Minimal non-isotypic supergroups

I [2] $pban$ (39); [2] $pbaa$ (43); [2] $pbam$ (44); [2] $p4bm$ (56); [2] $p\bar{4}b2$ (60)

II [2] $cmm2$ (26); [2] $pma2$ ($\mathbf{b}' = \frac{1}{2}\mathbf{b}$) (24)