

$pb a 2$

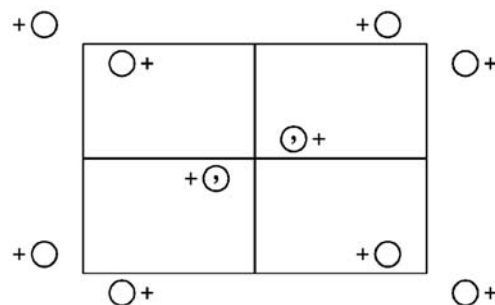
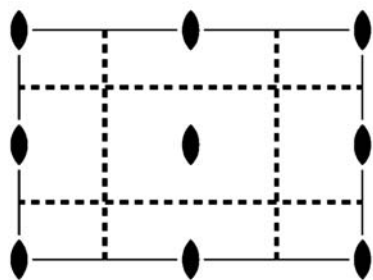
$mm 2$

Orthorhombic/Rectangular

No. 25

$pb a 2$

Patterson symmetry  $pmm m$



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) $b_{\frac{1}{4}, y, z}$         |
| $(1 0,0,0)$ | $(2_z 0,0,0)$   | $(m_y \frac{1}{2}, \frac{1}{2}, 0)$ | $(m_x \frac{1}{2}, \frac{1}{2}, 0)$ |

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

**Positions**

Multiplicity, Wyckoff letter, Site symmetry		Coordinates				Reflection conditions
4	<i>c</i> 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	<i>b</i> .. 2	$0, \frac{1}{2}, z$	$\frac{1}{2}, 0, z$			$hk: h + k = 2n$
2	<i>a</i> .. 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)