

$Pca2_1$

$C_{2v}^5$

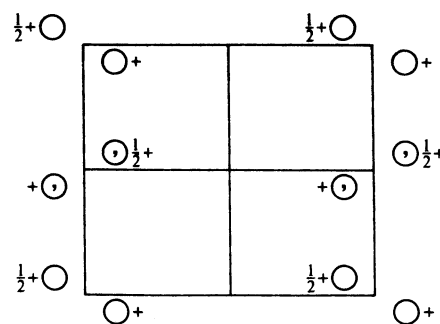
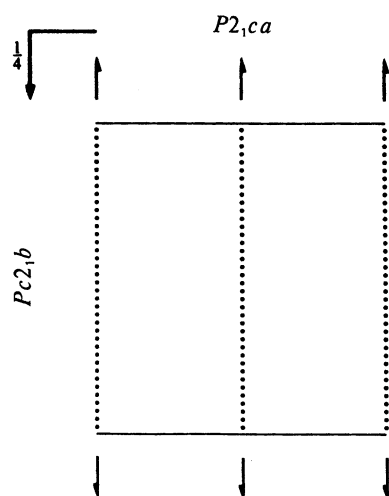
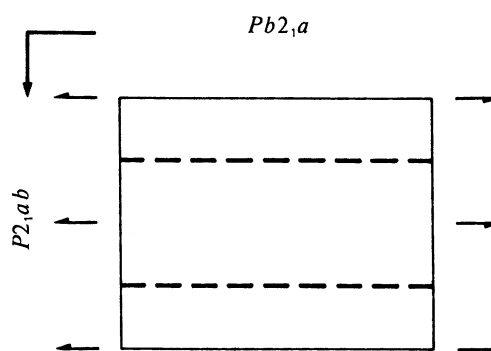
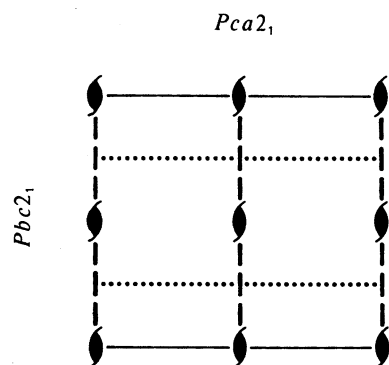
$mm2$

Orthorhombic

No. 29

$Pca2_1$

Patterson symmetry  $Pmmm$



Origin on  $1a2_1$

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

Symmetry operations

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

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

**Positions**

Multiplicity, Wyckoff letter, Site symmetry	Coordinates				Reflection conditions
					<b>General:</b>
4 <i>a</i> 1	(1) $x, y, z$	(2) $\bar{x}, \bar{y}, z + \frac{1}{2}$	(3) $x + \frac{1}{2}, \bar{y}, z$	(4) $\bar{x} + \frac{1}{2}, y, z + \frac{1}{2}$	$0kl : l = 2n$ $h0l : h = 2n$ $h00 : h = 2n$ $00l : l = 2n$

**Symmetry of special projections**

Along [001]  $p2mg$

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

Origin at 0, 0,  $z$

Along [100]  $p1m1$

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

Origin at  $x, 0, 0$

Along [010]  $p11g$

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

Origin at 0,  $y, 0$

**Maximal non-isomorphic subgroups**

**I**    [2]  $P1a1$  ( $Pc$ , 7)    1; 3  
       [2]  $Pc11$  ( $Pc$ , 7)    1; 4  
       [2]  $P112_1$  ( $P2_1$ , 4)    1; 2

**IIa** none

**IIb** [2]  $Pna2_1$  ( $\mathbf{b}' = 2\mathbf{b}$ ) (33)

**Maximal isomorphic subgroups of lowest index**

**IIc** [2]  $Pca2_1$  ( $\mathbf{b}' = 2\mathbf{b}$ ) (29); [3]  $Pca2_1$  ( $\mathbf{a}' = 3\mathbf{a}$ ) (29); [3]  $Pca2_1$  ( $\mathbf{c}' = 3\mathbf{c}$ ) (29)

**Minimal non-isomorphic supergroups**

**I**    [2]  $Pcca$  (54); [2]  $Pbcm$  (57); [2]  $Pbcn$  (60); [2]  $Pbca$  (61)

**II**    [2]  $Ccm2_1$  ( $Cmc2_1$ , 36); [2]  $Bme2$  ( $Aem2$ , 39); [2]  $Aea2$  (41); [2]  $Iba2$  (45); [2]  $Pcm2_1$  ( $\mathbf{a}' = \frac{1}{2}\mathbf{a}$ ) ( $Pmc2_1$ , 26);  
       [2]  $Pma2$  ( $\mathbf{c}' = \frac{1}{2}\mathbf{c}$ ) (28)