

$P\bar{4}$

$S_4^1$

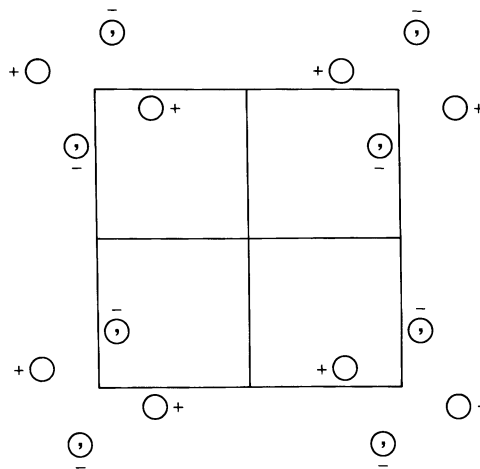
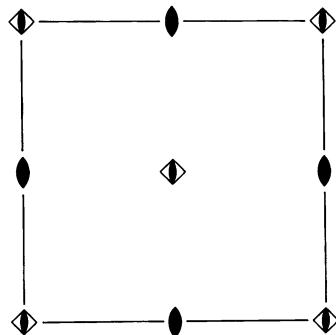
$\bar{4}$

Tetragonal

No. 81

$P\bar{4}$

Patterson symmetry  $P4/m$



Origin at  $\bar{4}$

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

Symmetry operations

- (1) 1            (2)  $2 \ 0,0,z$             (3)  $\bar{4}^+ \ 0,0,z; 0,0,0$             (4)  $\bar{4}^- \ 0,0,z; 0,0,0$

**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
4 $h$ 1	(1) $x, y, z$ (2) $\bar{x}, \bar{y}, z$ (3) $y, \bar{x}, \bar{z}$ (4) $\bar{y}, x, \bar{z}$	General: no conditions  Special:
2 $g$ 2..	$0, \frac{1}{2}, z$ $\frac{1}{2}, 0, \bar{z}$	$hk0 : h + k = 2n$
2 $f$ 2..	$\frac{1}{2}, \frac{1}{2}, z$ $\frac{1}{2}, \frac{1}{2}, \bar{z}$	no extra conditions
2 $e$ 2..	$0, 0, z$ $0, 0, \bar{z}$	no extra conditions
1 $d$ $\bar{4}$ ..	$\frac{1}{2}, \frac{1}{2}, \frac{1}{2}$	no extra conditions
1 $c$ $\bar{4}$ ..	$\frac{1}{2}, \frac{1}{2}, 0$	no extra conditions
1 $b$ $\bar{4}$ ..	$0, 0, \frac{1}{2}$	no extra conditions
1 $a$ $\bar{4}$ ..	$0, 0, 0$	no extra conditions

**Symmetry of special projections**

Along  $[001]$   $p4$   
 $\mathbf{a}' = \mathbf{a}$      $\mathbf{b}' = \mathbf{b}$   
 Origin at  $0, 0, z$

Along  $[100]$   $p1m1$   
 $\mathbf{a}' = \mathbf{b}$      $\mathbf{b}' = \mathbf{c}$   
 Origin at  $x, 0, 0$

Along  $[110]$   $p1m1$   
 $\mathbf{a}' = \frac{1}{2}(-\mathbf{a} + \mathbf{b})$      $\mathbf{b}' = \mathbf{c}$   
 Origin at  $x, x, 0$

**Maximal non-isomorphic subgroups**

**I**     $[2] P2(3)$     1; 2

**IIa**    none

**IIb**     $[2] F\bar{4} (\mathbf{a}' = 2\mathbf{a}, \mathbf{b}' = 2\mathbf{b}, \mathbf{c}' = 2\mathbf{c}) (I\bar{4}, 82)$

**Maximal isomorphic subgroups of lowest index**

**IIc**     $[2] P\bar{4} (\mathbf{c}' = 2\mathbf{c}) (81)$ ;  $[2] C\bar{4} (\mathbf{a}' = 2\mathbf{a}, \mathbf{b}' = 2\mathbf{b}) (P\bar{4}, 81)$

**Minimal non-isomorphic supergroups**

**I**     $[2] P4/m (83)$ ;  $[2] P4_2/m (84)$ ;  $[2] P4/n (85)$ ;  $[2] P4_2/n (86)$ ;  $[2] P\bar{4}2m (111)$ ;  $[2] P\bar{4}2c (112)$ ;  $[2] P\bar{4}2_1m (113)$ ;  $[2] P\bar{4}2_1c (114)$ ;  
 $[2] P\bar{4}m2 (115)$ ;  $[2] P\bar{4}c2 (116)$ ;  $[2] P\bar{4}b2 (117)$ ;  $[2] P\bar{4}n2 (118)$

**II**     $[2] I\bar{4} (82)$