

$P3_112$

$D_3^3$

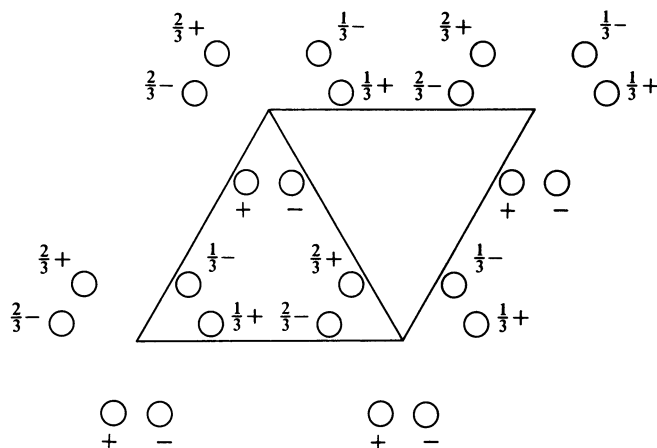
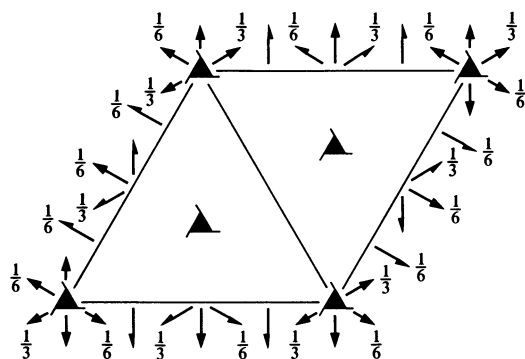
312

Trigonal

No. 151

$P3_112$

Patterson symmetry  $P\bar{3}1m$



Origin on  $2[210]$  at  $3_11(1,1,2)$

Asymmetric unit  $0 \leq x \leq 1; 0 \leq y \leq 1; 0 \leq z \leq \frac{1}{6}$   
 Vertices  $0,0,0$   $1,0,0$   $1,1,0$   $0,1,0$   
 $0,0,\frac{1}{6}$   $1,0,\frac{1}{6}$   $1,1,\frac{1}{6}$   $0,1,\frac{1}{6}$

Symmetry operations

- (1) 1 (2)  $3^+(0,0,\frac{1}{3})$   $0,0,z$  (3)  $3^-(0,0,\frac{2}{3})$   $0,0,z$   
 (4) 2  $x,\bar{x},\frac{1}{3}$  (5) 2  $x,2x,\frac{1}{6}$  (6) 2  $2x,x,0$

**Generators selected** (1);  $t(1,0,0)$ ;  $t(0,1,0)$ ;  $t(0,0,1)$ ; (2); (4)

**Positions**

Multiplicity, Wyckoff letter, Site symmetry	Coordinates			Reflection conditions
				General:
6 <i>c</i> 1	(1) $x, y, z$ (4) $\bar{y}, \bar{x}, \bar{z} + \frac{2}{3}$	(2) $\bar{y}, x - y, z + \frac{1}{3}$ (5) $\bar{x} + y, y, \bar{z} + \frac{1}{3}$	(3) $\bar{x} + y, \bar{x}, z + \frac{2}{3}$ (6) $x, x - y, \bar{z}$	$000l : l = 3n$
				Special: no extra conditions
3 <i>b</i> .. 2	$x, \bar{x}, \frac{5}{6}$	$x, 2x, \frac{1}{6}$	$2\bar{x}, \bar{x}, \frac{1}{2}$	
3 <i>a</i> .. 2	$x, \bar{x}, \frac{1}{3}$	$x, 2x, \frac{2}{3}$	$2\bar{x}, \bar{x}, 0$	

**Symmetry of special projections**

Along [001]  $P3m1$

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

Origin at 0, 0, z

Along [100]  $P11m$

$$\mathbf{a}' = \frac{1}{2}(\mathbf{a} + 2\mathbf{b}) \quad \mathbf{b}' = \mathbf{c}$$

Origin at  $x, 0, \frac{1}{6}$

Along [210]  $P2$

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

Origin at  $x, \frac{1}{2}x, 0$

**Maximal non-isomorphic subgroups**

<b>I</b>	[2] $P3_111$ ( $P3_1, 144$ )	1; 2; 3
	{ [3] $P112$ ( $C2, 5$ )	1; 4
	{ [3] $P112$ ( $C2, 5$ )	1; 5
	{ [3] $P112$ ( $C2, 5$ )	1; 6

**IIa** none

**IIb** [3]  $H3_112$  ( $\mathbf{a}' = 3\mathbf{a}, \mathbf{b}' = 3\mathbf{b}$ ) ( $P3, 21, 152$ )

**Maximal isomorphic subgroups of lowest index**

**IIc** [2]  $P3_212$  ( $\mathbf{c}' = 2\mathbf{c}$ ) (153); [4]  $P3_112$  ( $\mathbf{a}' = 2\mathbf{a}, \mathbf{b}' = 2\mathbf{b}$ ) (151); [7]  $P3_112$  ( $\mathbf{c}' = 7\mathbf{c}$ ) (151)

**Minimal non-isomorphic supergroups**

**I** [2]  $P6_122$  (178); [2]  $P6_422$  (181)

**II** [3]  $H3_112$  ( $P3_121, 152$ ); [3]  $P312$  ( $\mathbf{c}' = \frac{1}{3}\mathbf{c}$ ) (149)