

$P3_121$

D_3^4

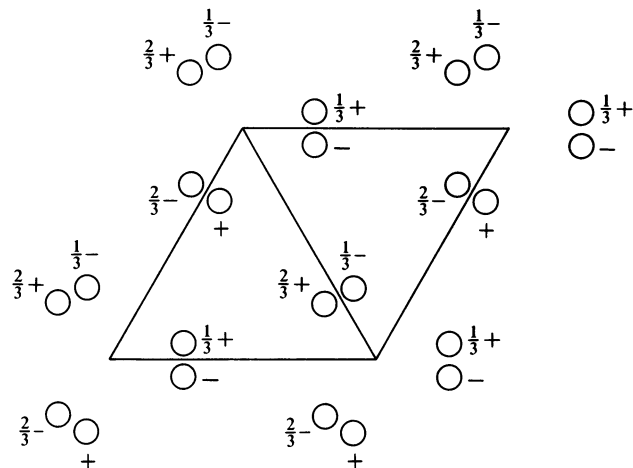
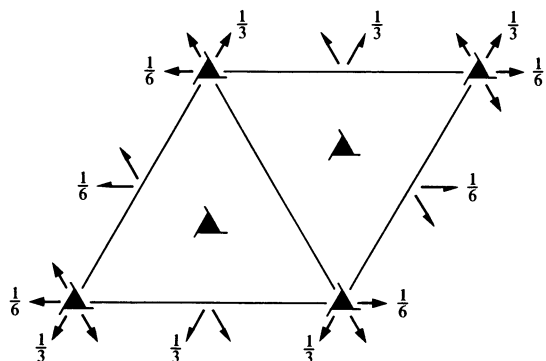
321

Trigonal

No. 152

$P3_121$

Patterson symmetry $P\bar{3}m1$



Origin on $2[110]$ at $3_1(1,1,2)1$

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

Vertices $0,0,0 \quad 1,0,0 \quad 1,1,0 \quad 0,1,0$

$0,0,\frac{1}{6} \quad 1,0,\frac{1}{6} \quad 1,1,\frac{1}{6} \quad 0,1,\frac{1}{6}$

Symmetry operations

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

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

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

General:

$000l : l = 3n$

Special: no extra conditions

3 b .2. $x, 0, \frac{5}{6}$ $0, x, \frac{1}{6}$ $\bar{x}, \bar{x}, \frac{1}{2}$

3 a .2. $x, 0, \frac{1}{3}$ $0, x, \frac{2}{3}$ $\bar{x}, \bar{x}, 0$

Symmetry of special projections

Along [001] $p31m$

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

Origin at $0, 0, z$

Along [100] $p2$

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

Origin at $x, 0, \frac{1}{3}$

Along [210] $p11m$

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

Origin at $x, \frac{1}{2}x, \frac{1}{6}$

Maximal non-isomorphic subgroups

I [2] $P3_111$ ($P3_1, 144$) 1; 2; 3
 $\left\{ \begin{array}{l} [3] P121 (C2, 5) \quad 1; 4 \\ [3] P121 (C2, 5) \quad 1; 5 \\ [3] P121 (C2, 5) \quad 1; 6 \end{array} \right.$

IIa none

IIb [3] $H3_121$ ($\mathbf{a}' = 3\mathbf{a}, \mathbf{b}' = 3\mathbf{b}$) ($P3, 12, 151$)

Maximal isomorphic subgroups of lowest index

IIc [2] $P3_221$ ($\mathbf{c}' = 2\mathbf{c}$) (154); [4] $P3_121$ ($\mathbf{a}' = 2\mathbf{a}, \mathbf{b}' = 2\mathbf{b}$) (152); [7] $P3_121$ ($\mathbf{c}' = 7\mathbf{c}$) (152)

Minimal non-isomorphic supergroups

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

II [3] $H3_121$ ($P3_1, 12, 151$); [3] $R32$ (obverse) (155); [3] $R32$ (reverse) (155); [3] $P321$ ($\mathbf{c}' = \frac{1}{3}\mathbf{c}$) (150)