

$P6_1$

$C_6^2$

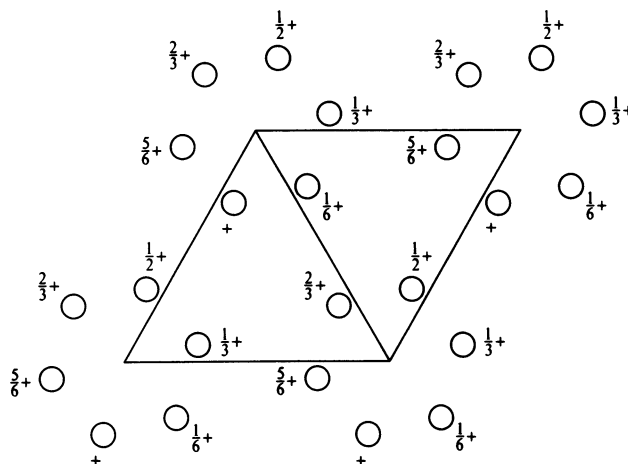
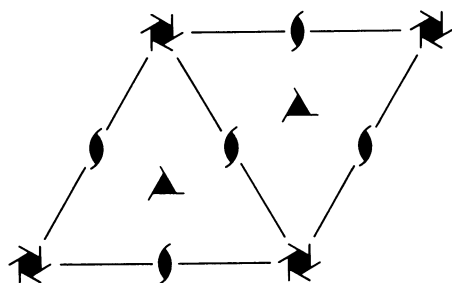
6

Hexagonal

No. 169

$P6_1$

Patterson symmetry  $P6/m$



Origin on  $6_1$

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

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 <i>a</i> 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) $\bar{x}, \bar{y}, z + \frac{1}{2}$ (5) $y, \bar{x} + y, z + \frac{5}{6}$ (6) $x - y, x, z + \frac{1}{6}$	General: $000l : l = 6n$

Symmetry of special projections

Along  $[001]$   $p6$   
 $\mathbf{a}' = \mathbf{a}$   $\mathbf{b}' = \mathbf{b}$   
 Origin at  $0, 0, z$

Along  $[100]$   $p1g1$   
 $\mathbf{a}' = \frac{1}{2}(\mathbf{a} + 2\mathbf{b})$   $\mathbf{b}' = \mathbf{c}$   
 Origin at  $x, 0, 0$

Along  $[210]$   $p1g1$   
 $\mathbf{a}' = \frac{1}{2}\mathbf{b}$   $\mathbf{b}' = \mathbf{c}$   
 Origin at  $x, \frac{1}{2}x, 0$

Maximal non-isomorphic subgroups

I  $[2]P3_1(144)$  1; 2; 3  
 $[3]P2_1(4)$  1; 4

IIa none

IIb none

Maximal isomorphic subgroups of lowest index

IIc  $[3]H6_1(\mathbf{a}' = 3\mathbf{a}, \mathbf{b}' = 3\mathbf{b})(P6_1, 169)$ ;  $[5]P6_5(\mathbf{c}' = 5\mathbf{c})(170)$ ;  $[7]P6_1(\mathbf{c}' = 7\mathbf{c})(169)$

Minimal non-isomorphic supergroups

I  $[2]P6_122(178)$

II  $[2]P6_2(\mathbf{c}' = \frac{1}{2}\mathbf{c})(171)$ ;  $[3]P6_3(\mathbf{c}' = \frac{1}{3}\mathbf{c})(173)$