

$P6_3/m$

C_{6h}^2

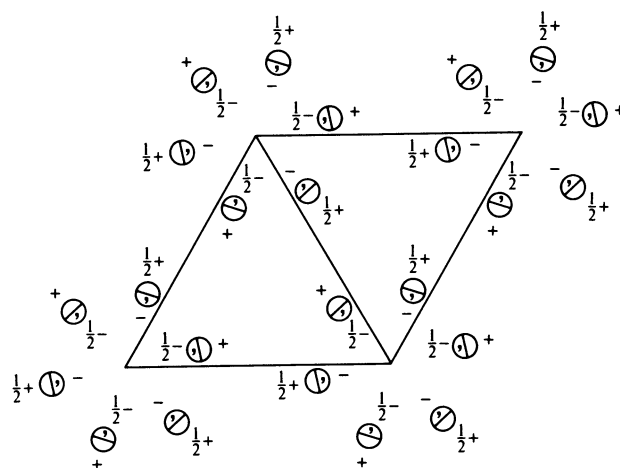
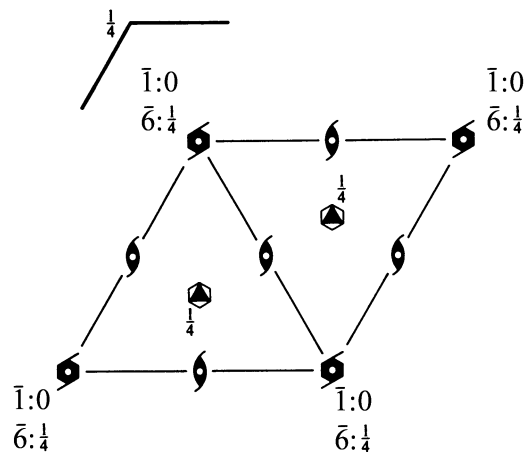
$6/m$

Hexagonal

No. 176

$P6_3/m$

Patterson symmetry $P6/m$



Origin at centre ($\bar{3}$) on 6_3

Asymmetric unit $0 \leq x \leq \frac{2}{3}; 0 \leq y \leq \frac{2}{3}; 0 \leq z \leq \frac{1}{4}; x \leq (1+y)/2; y \leq \min(1-x, (1+x)/2)$

Vertices $0, 0, 0$ $\frac{1}{2}, 0, 0$ $\frac{2}{3}, \frac{1}{3}, 0$ $\frac{1}{3}, \frac{2}{3}, 0$ $0, \frac{1}{2}, 0$
 $0, 0, \frac{1}{4}$ $\frac{1}{2}, 0, \frac{1}{4}$ $\frac{2}{3}, \frac{1}{3}, \frac{1}{4}$ $\frac{1}{3}, \frac{2}{3}, \frac{1}{4}$ $0, \frac{1}{2}, \frac{1}{4}$

Symmetry operations

- | | | |
|------------------------------------|---|---|
| (1) 1 | (2) $3^+ 0, 0, z$ | (3) $3^- 0, 0, z$ |
| (4) $2(0, 0, \frac{1}{2}) 0, 0, z$ | (5) $6^-(0, 0, \frac{1}{2}) 0, 0, z$ | (6) $6^+(0, 0, \frac{1}{2}) 0, 0, z$ |
| (7) $\bar{1} 0, 0, 0$ | (8) $\bar{3}^+ 0, 0, z; 0, 0, 0$ | (9) $\bar{3}^- 0, 0, z; 0, 0, 0$ |
| (10) $m x, y, \frac{1}{4}$ | (11) $\bar{6}^- 0, 0, z; 0, 0, \frac{1}{4}$ | (12) $\bar{6}^+ 0, 0, z; 0, 0, \frac{1}{4}$ |

Generators selected (1); $t(1,0,0)$; $t(0,1,0)$; $t(0,0,1)$; (2); (4); (7)

Positions

Multiplicity, Wyckoff letter, Site symmetry	Coordinates	Reflection conditions
12 <i>i</i> 1	(1) x, y, z (2) $\bar{y}, x - y, z$ (3) $\bar{x} + y, \bar{x}, z$ (4) $\bar{x}, \bar{y}, z + \frac{1}{2}$ (5) $y, \bar{x} + y, z + \frac{1}{2}$ (6) $x - y, x, z + \frac{1}{2}$ (7) $\bar{x}, \bar{y}, \bar{z}$ (8) $y, \bar{x} + y, \bar{z}$ (9) $x - y, x, \bar{z}$ (10) $x, y, \bar{z} + \frac{1}{2}$ (11) $\bar{y}, x - y, \bar{z} + \frac{1}{2}$ (12) $\bar{x} + y, \bar{x}, \bar{z} + \frac{1}{2}$	General: $000l : l = 2n$ Special: as above, plus
6 <i>h</i> $m..$	$x, y, \frac{1}{4}$ $\bar{y}, x - y, \frac{1}{4}$ $\bar{x} + y, \bar{x}, \frac{1}{4}$ $\bar{x}, \bar{y}, \frac{3}{4}$ $y, \bar{x} + y, \frac{3}{4}$ $x - y, x, \frac{3}{4}$	no extra conditions
6 <i>g</i> $\bar{1}$	$\frac{1}{2}, 0, 0$ $0, \frac{1}{2}, 0$ $\frac{1}{2}, \frac{1}{2}, 0$ $\frac{1}{2}, 0, \frac{1}{2}$ $0, \frac{1}{2}, \frac{1}{2}$ $\frac{1}{2}, \frac{1}{2}, \frac{1}{2}$	$hkil : l = 2n$
4 <i>f</i> $3..$	$\frac{1}{3}, \frac{2}{3}, z$ $\frac{2}{3}, \frac{1}{3}, z + \frac{1}{2}$ $\frac{2}{3}, \frac{1}{3}, \bar{z}$ $\frac{1}{3}, \frac{2}{3}, \bar{z} + \frac{1}{2}$	$hkil : l = 2n$ or $h - k = 3n + 1$ or $h - k = 3n + 2$
4 <i>e</i> $3..$	$0, 0, z$ $0, 0, z + \frac{1}{2}$ $0, 0, \bar{z}$ $0, 0, \bar{z} + \frac{1}{2}$	$hkil : l = 2n$
2 <i>d</i> $\bar{6}..$	$\frac{2}{3}, \frac{1}{3}, \frac{1}{4}$ $\frac{1}{3}, \frac{2}{3}, \frac{3}{4}$	$hkil : l = 2n$ or $h - k = 3n + 1$ or $h - k = 3n + 2$
2 <i>c</i> $\bar{6}..$	$\frac{1}{3}, \frac{2}{3}, \frac{1}{4}$ $\frac{2}{3}, \frac{1}{3}, \frac{3}{4}$	$hkil : l = 2n$ or $h - k = 3n + 1$ or $h - k = 3n + 2$
2 <i>b</i> $\bar{3}..$	$0, 0, 0$ $0, 0, \frac{1}{2}$	$hkil : l = 2n$
2 <i>a</i> $\bar{6}..$	$0, 0, \frac{1}{4}$ $0, 0, \frac{3}{4}$	$hkil : l = 2n$

Symmetry of special projections

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

Along [100] $p2gm$
 $\mathbf{a}' = \frac{1}{2}(\mathbf{a} + 2\mathbf{b})$ $\mathbf{b}' = \mathbf{c}$
Origin at $x, 0, 0$

Along [210] $p2gm$
 $\mathbf{a}' = \frac{1}{2}\mathbf{b}$ $\mathbf{b}' = \mathbf{c}$
Origin at $x, \frac{1}{2}x, 0$

Maximal non-isomorphic subgroups

I [2] $P\bar{6}$ (174) 1; 2; 3; 10; 11; 12
[2] $P6_3$ (173) 1; 2; 3; 4; 5; 6
[2] $P\bar{3}$ (147) 1; 2; 3; 7; 8; 9
[3] $P2_1/m$ (11) 1; 4; 7; 10

IIa none

IIb none

Maximal isomorphic subgroups of lowest index

IIc [3] $P6_3/m$ ($\mathbf{c}' = 3\mathbf{c}$) (176); [3] $H6_3/m$ ($\mathbf{a}' = 3\mathbf{a}, \mathbf{b}' = 3\mathbf{b}$) ($P6_3/m$, 176)

Minimal non-isomorphic supergroups

I [2] $P6_3/mcm$ (193); [2] $P6_3/mmc$ (194)

II [2] $P6/m$ ($\mathbf{c}' = \frac{1}{2}\mathbf{c}$) (175)