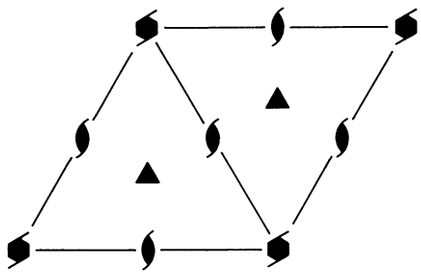
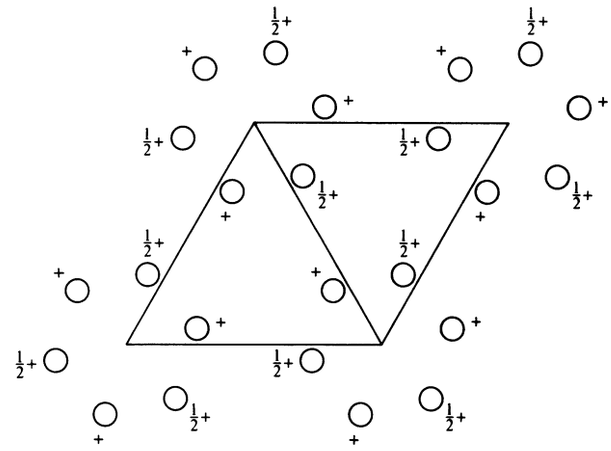
International Tables for Crystallography (2006). Vol. A, Space group 173, pp. 558–559.

$P6_3$ C_6^6 6 Hexagonal

No. 173 $P6_3$ Patterson symmetry $P6/m$





Origin on 3 on 6_3

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

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

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

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

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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	c	1	(1) x,y,z	(2) $\bar{y},x-y,z$	(3) $\bar{x}+y,\bar{x},z$	$000l$: $l=2n$
			(4) $\bar{x},\bar{y},z+\frac{1}{2}$	(5) $y,\bar{x}+y,z+\frac{1}{2}$	(6) $x-y,x,z+\frac{1}{2}$	
						Special: as above, plus
2	b	3 . .	$\frac{1}{3},\frac{2}{3},z$	$\frac{2}{3},\frac{1}{3},z+\frac{1}{2}$		$hkil$: $l=2n$ or $h-k=3n+1$ or $h-k=3n+2$
2	a	3 . .	$0,0,z$	$0,0,z+\frac{1}{2}$		$hkil$: $l=2n$

Symmetry of special projections

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

Along [100] $p1g1$
$\mathbf{a}'=\frac{1}{2}(\mathbf{a}+2\mathbf{b})$ $\mathbf{b}'=\mathbf{c}$
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] $P3$ (143) 1; 2; 3
[3] $P2_1$ (4) 1; 4

IIa none

IIb [3] $P6_5$ ($\mathbf{c}'=3\mathbf{c}$) (170); [3] $P6_1$ ($\mathbf{c}'=3\mathbf{c}$) (169)

Maximal isomorphic subgroups of lowest index

IIc [3] $P6_3$ ($\mathbf{c}'=3\mathbf{c}$) (173); [3] $H6_3$ ($\mathbf{a}'=3\mathbf{a},\mathbf{b}'=3\mathbf{b}$) ($P6_3$, 173)

Minimal non-isomorphic supergroups

I [2] $P6_3/m$ (176); [2] $P6_322$ (182); [2] $P6_3cm$ (185); [2] $P6_3mc$ (186)

II [2] $P6$ ($\mathbf{c}'=\frac{1}{2}\mathbf{c}$) (168)