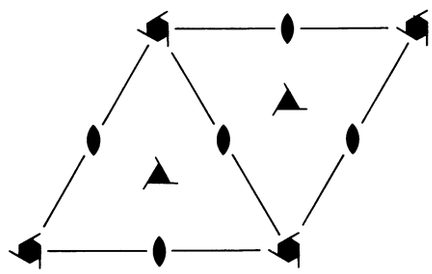
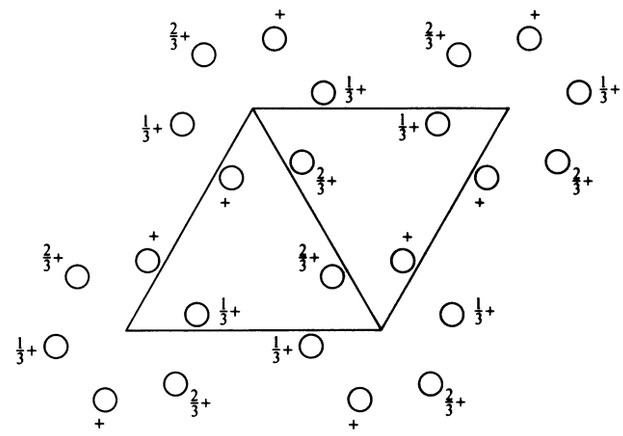
Hexagonal 6 C_6^5 $P6_4$

Patterson symmetry $P6/m$ $P6_4$ No. 172





Origin on 2 on 6_4

Asymmetric unit $0 \le x \le 1;\quad 0 \le y \le 1;\quad 0 \le z \le \frac{1}{3};\quad y \le x$

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

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

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

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

Symmetry of special projections

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

Along [100] $p1m1$
$\mathbf{a}'=\frac{1}{2}(\mathbf{a}+2\mathbf{b})$ $\mathbf{b}'=\mathbf{c}$
Origin at $x,0,0$

Along [210] $p1m1$
$\mathbf{a}'=\frac{1}{2}\mathbf{b}$ $\mathbf{b}'=\mathbf{c}$
Origin at $x,\frac{1}{2}x,0$

Maximal non-isomorphic subgroups

I [2] $P3_1$ (144) 1; 2; 3
[3] $P2$ (3) 1; 4

IIa none

IIb [2] $P6_5$ ($\mathbf{c}'=2\mathbf{c}$) (170)

Maximal isomorphic subgroups of lowest index

IIc [2] $P6_2$ ($\mathbf{c}'=2\mathbf{c}$) (171); [3] $H6_4$ ($\mathbf{a}'=3\mathbf{a},\mathbf{b}'=3\mathbf{b}$) ($P6_4$, 172); [7] $P6_4$ ($\mathbf{c}'=7\mathbf{c}$) (172)

Minimal non-isomorphic supergroups

I [2] $P6_422$ (181)

II [3] $P6$ ($\mathbf{c}'=\frac{1}{3}\mathbf{c}$) (168)

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