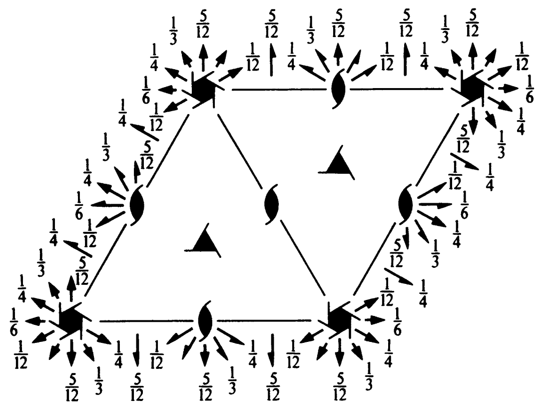
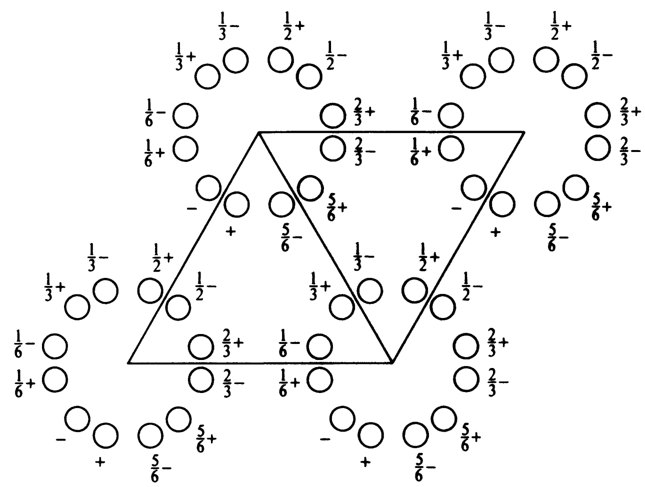
Hexagonal 622 D_6^3 $P6_522$

Patterson symmetry $P6/mmm$ $P6_522$ No. 179





Origin on $2[100]$ at $6_5\,(2,1,1)\,1$

Asymmetric unit $0 \le x \le 1;\quad 0 \le y \le 1;\quad 0 \le z \le \frac{1}{12}$

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

$0,0,\frac{1}{12} \quad 1,0,\frac{1}{12} \quad 1,1,\frac{1}{12} \quad 0,1,\frac{1}{12}$

Symmetry operations

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

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
							General:
12 c 1	(1) x,y,z	(2) $\bar{y},x-y,z+\frac{2}{3}$	(3) $\bar{x}+y,\bar{x},z+\frac{1}{3}$				$000l$: $l=6n$
	(4) $\bar{x},\bar{y},z+\frac{1}{2}$	(5) $y,\bar{x}+y,z+\frac{1}{6}$	(6) $x-y,x,z+\frac{5}{6}$				
	(7) $y,x,\bar{z}+\frac{2}{3}$	(8) $x-y,\bar{y},\bar{z}$	(9) $\bar{x},\bar{x}+y,\bar{z}+\frac{1}{3}$				
	(10) $\bar{y},\bar{x},\bar{z}+\frac{1}{6}$	(11) $\bar{x}+y,y,\bar{z}+\frac{1}{2}$	(12) $x,x-y,\bar{z}+\frac{5}{6}$				
							Special: as above, plus
6 b $..2$	$x,2x,\frac{3}{4}$	$2\bar{x},\bar{x},\frac{5}{12}$	$x,\bar{x},\frac{1}{12}$	$\bar{x},2\bar{x},\frac{1}{4}$	$2x,x,\frac{11}{12}$	$\bar{x},x,\frac{7}{12}$	$hh\overline{2h}l$: $l=2n$ or $l=3n+1$ or $l=3n+2$
6 a $.2.$	$x,0,0$	$0,x,\frac{2}{3}$	$\bar{x},\bar{x},\frac{1}{3}$	$\bar{x},0,\frac{1}{2}$	$0,\bar{x},\frac{1}{6}$	$x,x,\frac{5}{6}$	$h\bar{h}0l$: $l=2n$ or $l=3n+1$ or $l=3n+2$

Symmetry of special projections

Along [001] $p6mm$
$\mathbf{a}'=\mathbf{a}\quad \mathbf{b}'=\mathbf{b}$
Origin at $0,0,z$

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

Along [210] $p2gm$
$\mathbf{a}'=\frac{1}{2}\mathbf{b}\quad \mathbf{b}'=\mathbf{c}$
Origin at $x,\frac{1}{2}x,\frac{5}{12}$

