$P6_3/mmc$ $\quad\quad D_{6h}^4$ $\quad\quad\quad$ $6/mmm$ $\quad\quad\quad$ Hexagonal

No. 194 $\quad\quad\quad\quad$ $P\,6_3/m\,2/m\,2/c$ $\quad\quad\quad$ Patterson symmetry $P6/mmm$
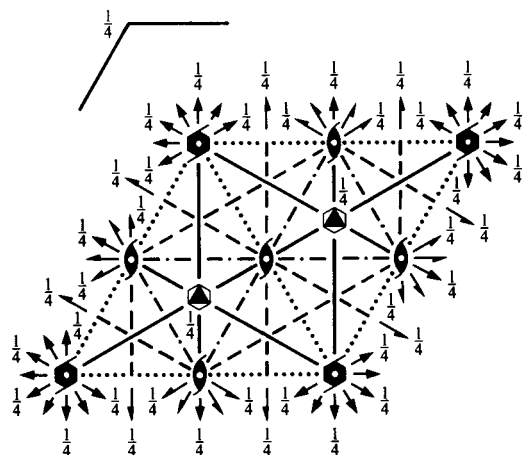
For $\bar{1}$ and $\bar{6}$ see $P6_3/m$ (No. 176)
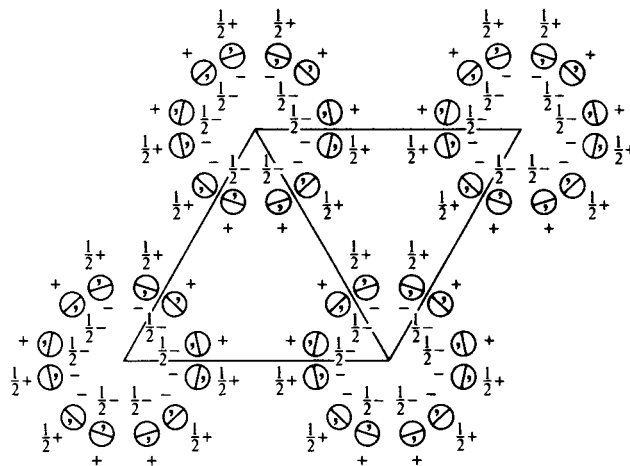
Origin at centre $(\bar{3}m1)$ at $\bar{3}2/mc$

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

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

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

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) 2 $x,x,0$	(8) 2 $x,0,0$	(9) 2 $0,y,0$
(10) 2 $x,\bar{x},\frac{1}{4}$	(11) 2 $x,2x,\frac{1}{4}$	(12) 2 $2x,x,\frac{1}{4}$
(13) $\bar{1}$ $0,0,0$	(14) $\bar{3}^+$ $0,0,z$; $0,0,0$	(15) $\bar{3}^-$ $0,0,z$; $0,0,0$
(16) m $x,y,\frac{1}{4}$	(17) $\bar{6}^-$ $0,0,z$; $0,0,\frac{1}{4}$	(18) $\bar{6}^+$ $0,0,z$; $0,0,\frac{1}{4}$
(19) m $x,\bar{x},z$	(20) m $x,2x,z$	(21) m $2x,x,z$
(22) c x,x,z	(23) c $x,0,z$	(24) c $0,y,z$

Maximal non-isomorphic subgroups

I $\quad$ [2] $P\bar{6}2c$ (190) $\quad\quad\quad\quad\quad\quad$ 1; 2; 3; 7; 8; 9; 16; 17; 18; 22; 23; 24

$\quad\quad$ [2] $P\bar{6}m2$ (187) $\quad\quad\quad\quad\quad\quad$ 1; 2; 3; 10; 11; 12; 16; 17; 18; 19; 20; 21

$\quad\quad$ [2] $P6_3mc$ (186) $\quad\quad\quad\quad\quad\quad$ 1; 2; 3; 4; 5; 6; 19; 20; 21; 22; 23; 24

$\quad\quad$ [2] $P6_322$ (182) $\quad\quad\quad\quad\quad\quad$ 1; 2; 3; 4; 5; 6; 7; 8; 9; 10; 11; 12

$\quad\quad$ [2] $P6_3/m11$ ($P6_3/m$, 176) $\quad$ 1; 2; 3; 4; 5; 6; 13; 14; 15; 16; 17; 18

$\quad\quad$ [2] $P\bar{3}m1$ (164) $\quad\quad\quad\quad\quad\quad$ 1; 2; 3; 7; 8; 9; 13; 14; 15; 19; 20; 21

$\quad\quad$ [2] $P\bar{3}1c$ (163) $\quad\quad\quad\quad\quad\quad$ 1; 2; 3; 10; 11; 12; 13; 14; 15; 22; 23; 24

$\quad\quad$ $\begin{cases} \text{[3] } Pmmc\,(Cmcm, 63) \\ \text{[3] } Pmmc\,(Cmcm, 63) \\ \text{[3] } Pmmc\,(Cmcm, 63) \end{cases}$ $\quad\quad$ 1; 4; 7; 10; 13; 16; 19; 22
$\quad\quad\quad\quad\quad\quad\quad\quad\quad\quad\quad\quad\quad\quad\quad$ 1; 4; 8; 11; 13; 16; 20; 23
$\quad\quad\quad\quad\quad\quad\quad\quad\quad\quad\quad\quad\quad\quad\quad$ 1; 4; 9; 12; 13; 16; 21; 24

IIa $\quad$ none

IIb $\quad$ [3] $H6_3/mmc$ ($\mathbf{a}'=3\mathbf{a}, \mathbf{b}'=3\mathbf{b}$) ($P6_3/mcm$, 193)

Maximal isomorphic subgroups of lowest index

IIc $\quad$ [3] $P6_3/mmc$ ($\mathbf{c}'=3\mathbf{c}$) (194); [4] $P6_3/mmc$ ($\mathbf{a}'=2\mathbf{a}, \mathbf{b}'=2\mathbf{b}$) (194)

Minimal non-isomorphic supergroups

I $\quad$ none

II $\quad$ [3] $H6_3/mmc$ ($P6_3/mcm$, 193); [2] $P6/mmm$ ($\mathbf{c}'=\frac{1}{2}\mathbf{c}$) (191)

Generators selected   (1); $t(1,0,0)$; $t(0,1,0)$; $t(0,0,1)$; (2); (4); (7); (13)

Positions

Multiplicity, Wyckoff letter, Site symmetry	Coordinates	Reflection conditions

General:

24	l	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) $y,x,\bar{z}$ (8) $x-y,\bar{y},\bar{z}$ (9) $\bar{x},\bar{x}+y,\bar{z}$
(10) $\bar{y},\bar{x},\bar{z}+\frac{1}{2}$ (11) $\bar{x}+y,y,\bar{z}+\frac{1}{2}$ (12) $x,x-y,\bar{z}+\frac{1}{2}$
(13) $\bar{x},\bar{y},\bar{z}$ (14) $y,\bar{x}+y,\bar{z}$ (15) $x-y,x,\bar{z}$
(16) $x,y,\bar{z}+\frac{1}{2}$ (17) $\bar{y},x-y,\bar{z}+\frac{1}{2}$ (18) $\bar{x}+y,\bar{x},\bar{z}+\frac{1}{2}$
(19) $\bar{y},\bar{x},z$ (20) $\bar{x}+y,y,z$ (21) $x,x-y,z$
(22) $y,x,z+\frac{1}{2}$ (23) $x-y,\bar{y},z+\frac{1}{2}$ (24) $\bar{x},\bar{x}+y,z+\frac{1}{2}$

$hh\overline{2h}l$: $l=2n$
$000l$: $l=2n$

Special: as above, plus

12	k	$.m.$	$x,2x,z$ $2\bar{x},\bar{x},z$ $x,\bar{x},z$ $\bar{x},2\bar{x},z+\frac{1}{2}$ $2x,x,z+\frac{1}{2}$ $\bar{x},x,z+\frac{1}{2}$ $2x,x,\bar{z}$ $\bar{x},2\bar{x},\bar{z}$ $\bar{x},x,\bar{z}$ $2\bar{x},\bar{x},\bar{z}+\frac{1}{2}$ $x,2x,\bar{z}+\frac{1}{2}$ $x,\bar{x},\bar{z}+\frac{1}{2}$	no extra conditions
12	j	$m..$	$x,y,\frac{1}{4}$ $\bar{y},x-y,\frac{1}{4}$ $\bar{x}+y,\bar{x},\frac{1}{4}$ $\bar{x},\bar{y},\frac{3}{4}$ $y,\bar{x}+y,\frac{3}{4}$ $x-y,x,\frac{3}{4}$ $y,x,\frac{3}{4}$ $x-y,\bar{y},\frac{3}{4}$ $\bar{x},\bar{x}+y,\frac{3}{4}$ $\bar{y},\bar{x},\frac{1}{4}$ $\bar{x}+y,y,\frac{1}{4}$ $x,x-y,\frac{1}{4}$	no extra conditions
12	i	$.2.$	$x,0,0$ $0,x,0$ $\bar{x},\bar{x},0$ $\bar{x},0,\frac{1}{2}$ $0,\bar{x},\frac{1}{2}$ $x,x,\frac{1}{2}$ $\bar{x},0,0$ $0,\bar{x},0$ $x,x,0$ $x,0,\frac{1}{2}$ $0,x,\frac{1}{2}$ $\bar{x},\bar{x},\frac{1}{2}$	$hkil$: $l=2n$
6	h	$mm2$	$x,2x,\frac{1}{4}$ $2\bar{x},\bar{x},\frac{1}{4}$ $x,\bar{x},\frac{1}{4}$ $\bar{x},2\bar{x},\frac{3}{4}$ $2x,x,\frac{3}{4}$ $\bar{x},x,\frac{3}{4}$	no extra conditions
6	g	$.2/m.$	$\frac{1}{2},0,0$ $0,\frac{1}{2},0$ $\frac{1}{2},\frac{1}{2},0$ $\frac{1}{2},0,\frac{1}{2}$ $0,\frac{1}{2},\frac{1}{2}$ $\frac{1}{2},\frac{1}{2},\frac{1}{2}$	$hkil$: $l=2n$
4	f	$3m.$	$\frac{1}{3},\frac{2}{3},z$ $\frac{2}{3},\frac{1}{3},z+\frac{1}{2}$ $\frac{2}{3},\frac{1}{3},\bar{z}$ $\frac{1}{3},\frac{2}{3},\bar{z}+\frac{1}{2}$	$hkil$: $l=2n$ or $h-k=3n+1$ or $h-k=3n+2$
4	e	$3m.$	$0,0,z$ $0,0,z+\frac{1}{2}$ $0,0,\bar{z}$ $0,0,\bar{z}+\frac{1}{2}$	$hkil$: $l=2n$
2	d	$\bar{6}m2$	$\frac{1}{3},\frac{2}{3},\frac{3}{4}$ $\frac{2}{3},\frac{1}{3},\frac{1}{4}$ $\Big\}$	$hkil$: $l=2n$ or $h-k=3n+1$ or $h-k=3n+2$
2	c	$\bar{6}m2$	$\frac{1}{3},\frac{2}{3},\frac{1}{4}$ $\frac{2}{3},\frac{1}{3},\frac{3}{4}$	
2	b	$\bar{6}m2$	$0,0,\frac{1}{4}$ $0,0,\frac{3}{4}$	$hkil$: $l=2n$
2	a	$\bar{3}m.$	$0,0,0$ $0,0,\frac{1}{2}$	$hkil$: $l=2n$

Symmetry of special projections

Along [001] $p6mm$
$\mathbf{a}'=\mathbf{a}$ $\mathbf{b}'=\mathbf{b}$
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] $p2mm$
$\mathbf{a}'=\frac{1}{2}\mathbf{b}$ $\mathbf{b}'=\frac{1}{2}\mathbf{c}$
Origin at $x,\frac{1}{2}x,0$