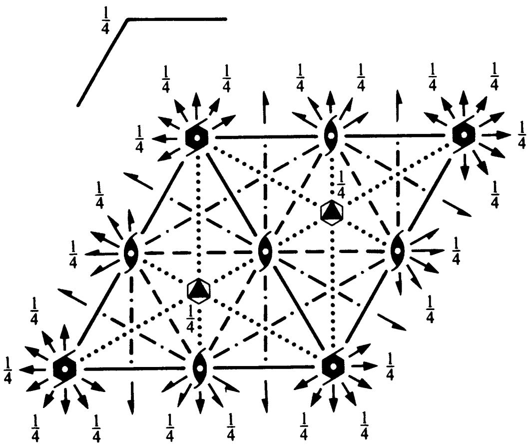
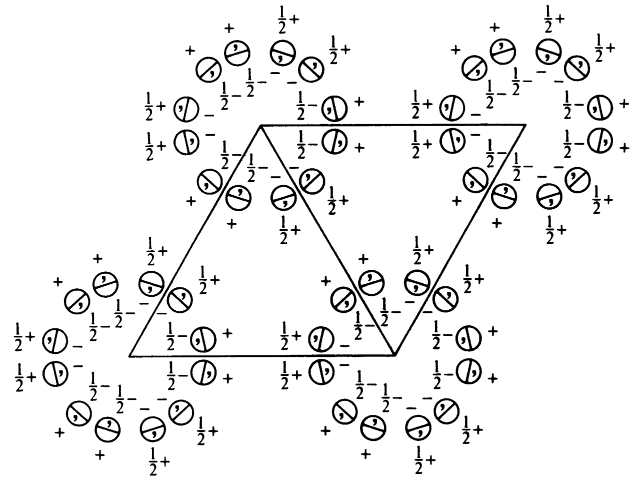
International Tables for Crystallography (2006). Vol. A, Space group 193, pp. 598–599.

$P6_3/mcm$ $\quad D_{6h}^3$ $\quad 6/mmm$ $\quad$ Hexagonal

No. 193 $\quad P\;6_3/m\;2/c\;2/m$ $\quad$ Patterson symmetry $P6/mmm$



For $\bar{1}$ and $\bar{6}$ see $P6_3/m$ (No. 176)



Origin at centre ($\bar{3}1m$) at $\bar{3}c2/m$

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

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

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

Symmetry operations

(1) 1	(2) $3^+\ 0,0,z$	(3) $3^-\ 0,0,z$
(4) $2(0,0,\frac{1}{2})\quad 0,0,z$	(5) $6^-(0,0,\frac{1}{2})\quad 0,0,z$	(6) $6^+(0,0,\frac{1}{2})\quad 0,0,z$
(7) $2\quad x,x,\frac{1}{4}$	(8) $2\quad x,0,\frac{1}{4}$	(9) $2\quad 0,y,\frac{1}{4}$
(10) $2\quad x,\bar{x},0$	(11) $2\quad x,2x,0$	(12) $2\quad 2x,x,0$
(13) $\bar{1}\quad 0,0,0$	(14) $\bar{3}^+\ 0,0,z;\ 0,0,0$	(15) $\bar{3}^-\ 0,0,z;\ 0,0,0$
(16) $m\quad x,y,\frac{1}{4}$	(17) $\bar{6}^-\ 0,0,z;\ 0,0,\frac{1}{4}$	(18) $\bar{6}^+\ 0,0,z;\ 0,0,\frac{1}{4}$
(19) $c\quad x,\bar{x},z$	(20) $c\quad x,2x,z$	(21) $c\quad 2x,x,z$
(22) $m\quad x,x,z$	(23) $m\quad x,0,z$	(24) $m\quad 0,y,z$

Maximal non-isomorphic subgroups

I	[2] $P\bar{6}2m$ (189)	1; 2; 3; 7; 8; 9; 16; 17; 18; 22; 23; 24
	[2] $P\bar{6}c2$ (188)	1; 2; 3; 10; 11; 12; 16; 17; 18; 19; 20; 21
	[2] $P6_3cm$ (185)	1; 2; 3; 4; 5; 6; 19; 20; 21; 22; 23; 24
	[2] $P6_322$ (182)	1; 2; 3; 4; 5; 6; 7; 8; 9; 10; 11; 12
	[2] $P6_3/m11$ ($P6_3/m$, 176)	1; 2; 3; 4; 5; 6; 13; 14; 15; 16; 17; 18
	[2] $P\bar{3}c1$ (165)	1; 2; 3; 7; 8; 9; 13; 14; 15; 19; 20; 21
	[2] $P\bar{3}1m$ (162)	1; 2; 3; 10; 11; 12; 13; 14; 15; 22; 23; 24
	{ [3] $Pmcm$ ($Cmcm$, 63)	1; 4; 7; 10; 13; 16; 19; 22
	{ [3] $Pmcm$ ($Cmcm$, 63)	1; 4; 8; 11; 13; 16; 20; 23
	{ [3] $Pmcm$ ($Cmcm$, 63)	1; 4; 9; 12; 13; 16; 21; 24

IIa none

IIb [3] $H6_3/mcm$ ($\mathbf{a}' = 3\mathbf{a}, \mathbf{b}' = 3\mathbf{b}$) ($P6_3/mmc$, 194)

Maximal isomorphic subgroups of lowest index

IIc [3] $P6_3/mcm$ ($\mathbf{c}' = 3\mathbf{c}$) (193); [4] $P6_3/mcm$ ($\mathbf{a}' = 2\mathbf{a}, \mathbf{b}' = 2\mathbf{b}$) (193)

Minimal non-isomorphic supergroups

I none

II [3] $H6_3/mcm$ ($P6_3/mmc$, 194); [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) $y,x,\bar{z}+\frac{1}{2}$ (8) $x-y,\bar{y},\bar{z}+\frac{1}{2}$ (9) $\bar{x},\bar{x}+y,\bar{z}+\frac{1}{2}$ (10) $\bar{y},\bar{x},\bar{z}$ (11) $\bar{x}+y,y,\bar{z}$ (12) $x,x-y,\bar{z}$ (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) $\bar{y},\bar{x},z+\frac{1}{2}$ (20) $\bar{x}+y,y,z+\frac{1}{2}$ (21) $x,x-y,z+\frac{1}{2}$ (22) y,x,z (23) $x-y,\bar{y},z$ (24) $\bar{x},\bar{x}+y,z$	$h\bar{h}0l$: $l=2n$ $000l$: $l=2n$
				Special: as above, plus
12	k	$..m$	$x,0,z$ $0,x,z$ $\bar{x},\bar{x},z$ $\bar{x},0,z+\frac{1}{2}$ $0,\bar{x},z+\frac{1}{2}$ $x,x,z+\frac{1}{2}$ $0,x,\bar{z}+\frac{1}{2}$ $x,0,\bar{z}+\frac{1}{2}$ $\bar{x},\bar{x},\bar{z}+\frac{1}{2}$ $0,\bar{x},\bar{z}$ $\bar{x},0,\bar{z}$ $x,x,\bar{z}$	no extra conditions
12	j	$m..$	$x,y,\frac{1}{4}$ $\bar{y},x-y,\frac{1}{4}$ $\bar{x}+y,\bar{x},\frac{1}{4}$ $\bar{x},\bar{y},\frac{3}{4}$ $y,\bar{x}+y,\frac{3}{4}$ $x-y,x,\frac{3}{4}$ $y,x,\frac{1}{4}$ $x-y,\bar{y},\frac{1}{4}$ $\bar{x},\bar{x}+y,\frac{1}{4}$ $\bar{y},\bar{x},\frac{3}{4}$ $\bar{x}+y,y,\frac{3}{4}$ $x,x-y,\frac{3}{4}$	no extra conditions
12	i	$..2$	$x,2x,0$ $2\bar{x},\bar{x},0$ $x,\bar{x},0$ $\bar{x},2\bar{x},\frac{1}{2}$ $2x,x,\frac{1}{2}$ $\bar{x},x,\frac{1}{2}$ $\bar{x},2\bar{x},0$ $2x,x,0$ $\bar{x},x,0$ $x,2x,\frac{1}{2}$ $2\bar{x},\bar{x},\frac{1}{2}$ $x,\bar{x},\frac{1}{2}$	$hkil$: $l=2n$
8	h	$3..$	$\frac{1}{3},\frac{2}{3},z$ $\frac{2}{3},\frac{1}{3},z+\frac{1}{2}$ $\frac{2}{3},\frac{1}{3},\bar{z}+\frac{1}{2}$ $\frac{1}{3},\frac{2}{3},\bar{z}$ $\frac{2}{3},\frac{1}{3},\bar{z}$ $\frac{1}{3},\frac{2}{3},\bar{z}+\frac{1}{2}$ $\frac{1}{3},\frac{2}{3},z+\frac{1}{2}$ $\frac{2}{3},\frac{1}{3},z$	$hkil$: $l=2n$
6	g	$m2m$	$x,0,\frac{1}{4}$ $0,x,\frac{1}{4}$ $\bar{x},\bar{x},\frac{1}{4}$ $\bar{x},0,\frac{3}{4}$ $0,\bar{x},\frac{3}{4}$ $x,x,\frac{3}{4}$	no extra conditions
6	f	$..2/m$	$\frac{1}{2},0,0$ $0,\frac{1}{2},0$ $\frac{1}{2},\frac{1}{2},0$ $\frac{1}{2},0,\frac{1}{2}$ $0,\frac{1}{2},\frac{1}{2}$ $\frac{1}{2},\frac{1}{2},\frac{1}{2}$	$hkil$: $l=2n$
4	e	$3.m$	$0,0,z$ $0,0,z+\frac{1}{2}$ $0,0,\bar{z}+\frac{1}{2}$ $0,0,\bar{z}$	$hkil$: $l=2n$
4	d	3.2	$\frac{1}{3},\frac{2}{3},0$ $\frac{2}{3},\frac{1}{3},\frac{1}{2}$ $\frac{2}{3},\frac{1}{3},0$ $\frac{1}{3},\frac{2}{3},\frac{1}{2}$	$hkil$: $l=2n$
4	c	$\bar{6}..$	$\frac{1}{3},\frac{2}{3},\frac{1}{4}$ $\frac{2}{3},\frac{1}{3},\frac{3}{4}$ $\frac{2}{3},\frac{1}{3},\frac{1}{4}$ $\frac{1}{3},\frac{2}{3},\frac{3}{4}$	$hkil$: $l=2n$
2	b	$\bar{3}.m$	$0,0,0$ $0,0,\frac{1}{2}$	$hkil$: $l=2n$
2	a	$\bar{6}2m$	$0,0,\frac{1}{4}$ $0,0,\frac{3}{4}$	$hkil$: $l=2n$

Symmetry of special projections

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

Along [100] $p2mm$
$\mathbf{a}'=\frac{1}{2}(\mathbf{a}+2\mathbf{b})$ $\mathbf{b}'=\frac{1}{2}\mathbf{c}$
Origin at $x,0,0$

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

(*Continued on preceding page*)