

$P6_3/mmc$

D_{6h}^4

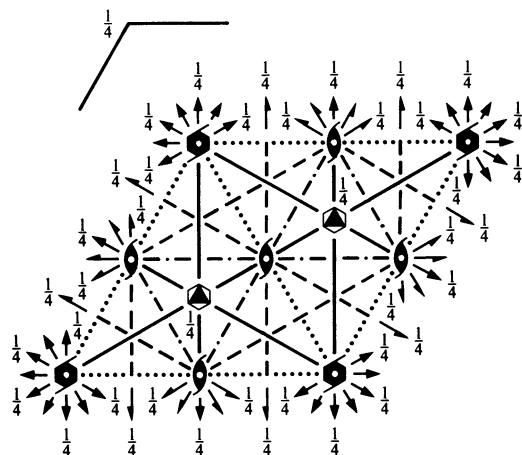
$6/mmm$

Hexagonal

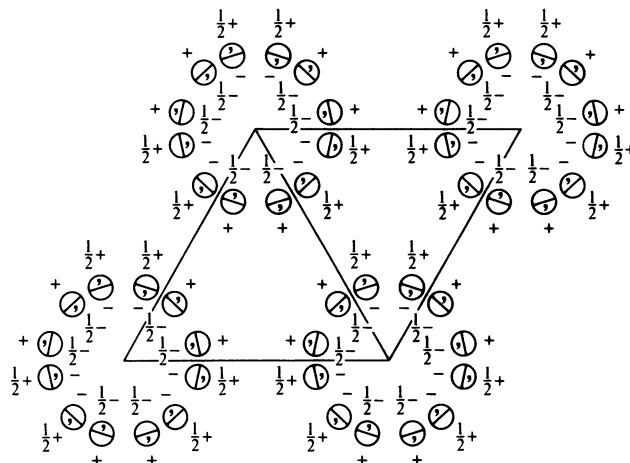
No. 194

$P 6_3/m 2/m 2/c$

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 $0 \leq x \leq \frac{2}{3}$; $0 \leq y \leq \frac{2}{3}$; $0 \leq z \leq \frac{1}{4}$; $x \leq 2y$; $y \leq \min(1-x, 2x)$

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

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** [2] $P\bar{6}2c$ (190) 1; 2; 3; 7; 8; 9; 16; 17; 18; 22; 23; 24
 [2] $P\bar{6}m2$ (187) 1; 2; 3; 10; 11; 12; 16; 17; 18; 19; 20; 21
 [2] $P6_3mc$ (186) 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] $P\bar{3}m1$ (164) 1; 2; 3; 7; 8; 9; 13; 14; 15; 19; 20; 21
 [2] $P\bar{3}1c$ (163) 1; 2; 3; 10; 11; 12; 13; 14; 15; 22; 23; 24
 { [3] $Pm\bar{6}c$ ($Cm\bar{6}c$, 63) 1; 4; 7; 10; 13; 16; 19; 22
 [3] $Pm\bar{6}c$ ($Cm\bar{6}c$, 63) 1; 4; 8; 11; 13; 16; 20; 23
 [3] $Pm\bar{6}c$ ($Cm\bar{6}c$, 63) 1; 4; 9; 12; 13; 16; 21; 24

IIa none

IIb [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 [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 none

II [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
24 <i>l</i> 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) $\bar{x}, \bar{x} + y, z + \frac{1}{2}$	General: $hh\bar{2}hl$: $l = 2n$ $000l$: $l = 2n$ Special: as above, plus no extra conditions
12 <i>k</i> . <i>m</i> .	$x, 2x, z$ $2x, x, z + \frac{1}{2}$ \bar{x}, x, \bar{z} $2\bar{x}, \bar{x}, z$ $\bar{x}, x, z + \frac{1}{2}$ $2\bar{x}, \bar{x}, \bar{z} + \frac{1}{2}$ x, \bar{x}, z $2x, x, \bar{z}$ $x, 2x, \bar{z} + \frac{1}{2}$ $\bar{x}, 2\bar{x}, z + \frac{1}{2}$ $\bar{x}, 2\bar{x}, \bar{z}$ $x, \bar{x}, \bar{z} + \frac{1}{2}$	no extra conditions
12 <i>j</i> <i>m</i> . .	$x, y, \frac{1}{4}$ $y, x, \frac{3}{4}$ $\bar{y}, x - y, \frac{1}{4}$ $x - y, \bar{y}, \frac{3}{4}$ $\bar{x} + y, \bar{x}, \frac{1}{4}$ $\bar{x}, \bar{x} + y, \frac{3}{4}$ $\bar{x}, \bar{y}, \frac{3}{4}$ $\bar{y}, \bar{x}, \frac{1}{4}$ $y, \bar{x} + y, \frac{3}{4}$ $\bar{x} + y, y, \frac{1}{4}$ $x - y, x, \frac{3}{4}$ $x, x - y, \frac{1}{4}$	no extra conditions
12 <i>i</i> . 2 .	$x, 0, 0$ $\bar{x}, 0, 0$ $0, x, 0$ $0, \bar{x}, 0$ $\bar{x}, \bar{x}, 0$ $x, x, 0$ $\bar{x}, 0, \frac{1}{2}$ $x, 0, \frac{1}{2}$ $0, \bar{x}, \frac{1}{2}$ $x, x, \frac{1}{2}$ $0, x, \frac{1}{2}$ $\bar{x}, \bar{x}, \frac{1}{2}$	$hkil$: $l = 2n$
6 <i>h</i> <i>m m</i> 2	$x, 2x, \frac{1}{4}$ $2\bar{x}, \bar{x}, \frac{1}{4}$ $x, \bar{x}, \frac{1}{4}$ $\bar{x}, 2\bar{x}, \frac{3}{4}$ $2x, x, \frac{3}{4}$ $\bar{x}, x, \frac{3}{4}$	no extra conditions
6 <i>g</i> . 2/ <i>m</i> .	$\frac{1}{2}, 0, 0$ $0, \frac{1}{2}, 0$ $\frac{1}{2}, \frac{1}{2}, 0$ $\frac{1}{2}, 0, \frac{1}{2}$ $0, \frac{1}{2}, \frac{1}{2}$ $\frac{1}{2}, \frac{1}{2}, \frac{1}{2}$	$hkil$: $l = 2n$
4 <i>f</i> 3 <i>m</i> .	$\frac{1}{3}, \frac{2}{3}, z$ $\frac{2}{3}, \frac{1}{3}, z + \frac{1}{2}$ $\frac{2}{3}, \frac{1}{3}, \bar{z}$ $\frac{1}{3}, \frac{2}{3}, \bar{z} + \frac{1}{2}$	$hkil$: $l = 2n$ or $h - k = 3n + 1$ or $h - k = 3n + 2$
4 <i>e</i> 3 <i>m</i> .	$0, 0, z$ $0, 0, z + \frac{1}{2}$ $0, 0, \bar{z}$ $0, 0, \bar{z} + \frac{1}{2}$	$hkil$: $l = 2n$
2 <i>d</i> $\bar{6}m2$	$\frac{1}{3}, \frac{2}{3}, \frac{3}{4}$ $\frac{2}{3}, \frac{1}{3}, \frac{1}{4}$	$hkil$: $l = 2n$ or $h - k = 3n + 1$ or $h - k = 3n + 2$
2 <i>c</i> $\bar{6}m2$	$\frac{1}{3}, \frac{2}{3}, \frac{1}{4}$ $\frac{2}{3}, \frac{1}{3}, \frac{3}{4}$	
2 <i>b</i> $\bar{6}m2$	$0, 0, \frac{1}{4}$ $0, 0, \frac{3}{4}$	$hkil$: $l = 2n$
2 <i>a</i> $\bar{3}m$.	$0, 0, 0$ $0, 0, \frac{1}{2}$	$hkil$: $l = 2n$

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

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