

$P6/mmm$

D_{6h}^1

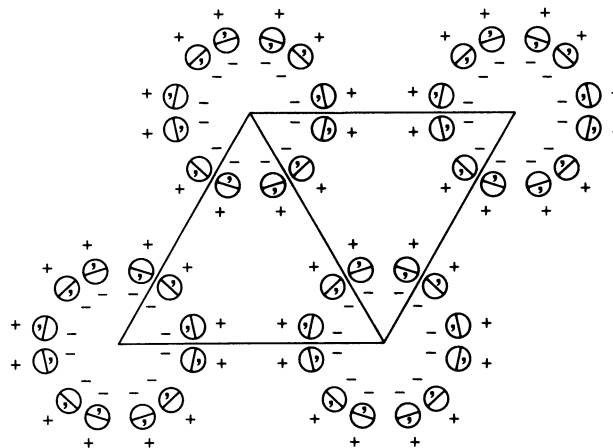
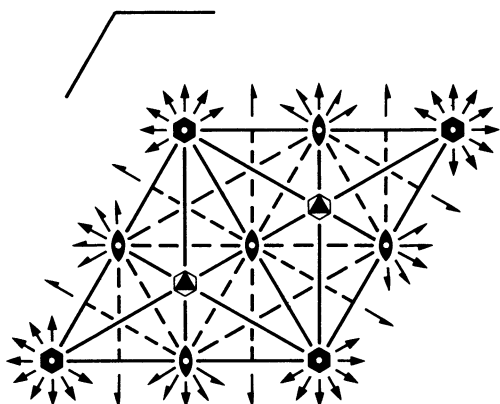
$6/mmm$

Hexagonal

No. 191

$P 6/m 2/m 2/m$

Patterson symmetry $P6/mmm$



Origin at centre ($6/mmm$)

Asymmetric unit $0 \leq x \leq \frac{2}{3}; 0 \leq y \leq \frac{1}{3}; 0 \leq z \leq \frac{1}{2}; x \leq (1+y)/2; y \leq x/2$

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

Symmetry operations

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

Maximal non-isomorphic subgroups

- I**
- | | |
|------------------------------|---|
| [2] $P\bar{6}2m$ (189) | 1; 2; 3; 7; 8; 9; 16; 17; 18; 22; 23; 24 |
| [2] $P\bar{6}m2$ (187) | 1; 2; 3; 10; 11; 12; 16; 17; 18; 19; 20; 21 |
| [2] $P6mm$ (183) | 1; 2; 3; 4; 5; 6; 19; 20; 21; 22; 23; 24 |
| [2] $P622$ (177) | 1; 2; 3; 4; 5; 6; 7; 8; 9; 10; 11; 12 |
| [2] $P6/m11$ ($P6/m$, 175) | 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] $P\bar{3}1m$ (162) | 1; 2; 3; 10; 11; 12; 13; 14; 15; 22; 23; 24 |
| { [3] $Pmmm$ ($Cmmm$, 65) | 1; 4; 7; 10; 13; 16; 19; 22 |
| { [3] $Pmmm$ ($Cmmm$, 65) | 1; 4; 8; 11; 13; 16; 20; 23 |
| { [3] $Pmmm$ ($Cmmm$, 65) | 1; 4; 9; 12; 13; 16; 21; 24 |

IIa none

IIb [2] $P6_3/mmc$ ($c' = 2c$) (194); [2] $P6_3/mcm$ ($c' = 2c$) (193); [2] $P6/mcc$ ($c' = 2c$) (192)

Maximal isomorphic subgroups of lowest index

IIc [2] $P6/mmm$ ($c' = 2c$) (191); [3] $H6/mmm$ ($a' = 3a, b' = 3b$) ($P6/mmm$, 191)

Minimal non-isomorphic supergroups

I none

II none

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	<i>r</i>	1	(1) x, y, z (4) \bar{x}, \bar{y}, z (7) y, x, \bar{z} (10) $\bar{y}, \bar{x}, \bar{z}$ (13) $\bar{x}, \bar{y}, \bar{z}$ (16) x, y, \bar{z} (19) \bar{y}, \bar{x}, z (22) y, x, z	(2) $\bar{y}, x - y, z$ (5) $y, \bar{x} + y, z$ (8) $x - y, \bar{y}, \bar{z}$ (11) $\bar{x} + y, y, \bar{z}$ (14) $y, \bar{x} + y, \bar{z}$ (17) $\bar{y}, x - y, \bar{z}$ (20) $\bar{x} + y, y, z$ (23) $x - y, \bar{y}, z$	(3) $\bar{x} + y, \bar{x}, z$ (6) $x - y, x, z$ (9) $\bar{x}, \bar{x} + y, \bar{z}$ (12) $x, x - y, \bar{z}$ (15) $x - y, x, \bar{z}$ (18) $\bar{x} + y, \bar{x}, \bar{z}$ (21) $x, x - y, z$ (24) $\bar{x}, \bar{x} + y, z$	no conditions
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Special: no extra conditions

12	<i>q</i>	<i>m . .</i>	$x, y, \frac{1}{2}$ $y, x, \frac{1}{2}$	$\bar{y}, x - y, \frac{1}{2}$ $x - y, \bar{y}, \frac{1}{2}$	$\bar{x} + y, \bar{x}, \frac{1}{2}$ $\bar{x}, \bar{x} + y, \frac{1}{2}$	$\bar{x}, \bar{y}, \frac{1}{2}$ $\bar{y}, \bar{x}, \frac{1}{2}$	$y, \bar{x} + y, \frac{1}{2}$ $\bar{x} + y, y, \frac{1}{2}$	$x - y, x, \frac{1}{2}$ $x, x - y, \frac{1}{2}$
12	<i>p</i>	<i>m . .</i>	$x, y, 0$ $y, x, 0$	$\bar{y}, x - y, 0$ $x - y, \bar{y}, 0$	$\bar{x} + y, \bar{x}, 0$ $\bar{x}, \bar{x} + y, 0$	$\bar{x}, \bar{y}, 0$ $\bar{y}, \bar{x}, 0$	$y, \bar{x} + y, 0$ $\bar{x} + y, y, 0$	$x - y, x, 0$ $x, x - y, 0$
12	<i>o</i>	<i>. m .</i>	$x, 2x, z$ $2x, x, \bar{z}$	$2\bar{x}, \bar{x}, z$ $\bar{x}, 2\bar{x}, \bar{z}$	x, \bar{x}, z \bar{x}, x, \bar{z}	$\bar{x}, 2\bar{x}, z$ $2\bar{x}, \bar{x}, \bar{z}$	$2x, x, z$ $x, 2x, \bar{z}$	\bar{x}, x, z x, \bar{x}, \bar{z}
12	<i>n</i>	<i>. . m</i>	$x, 0, z$ $0, x, \bar{z}$	$0, x, z$ $x, 0, \bar{z}$	\bar{x}, \bar{x}, z $\bar{x}, \bar{x}, \bar{z}$	$\bar{x}, 0, z$ $0, \bar{x}, \bar{z}$	$0, \bar{x}, z$ $\bar{x}, 0, \bar{z}$	x, x, z x, x, \bar{z}
6	<i>m</i>	<i>m m 2</i>	$x, 2x, \frac{1}{2}$	$2\bar{x}, \bar{x}, \frac{1}{2}$	$x, \bar{x}, \frac{1}{2}$	$\bar{x}, 2\bar{x}, \frac{1}{2}$	$2x, x, \frac{1}{2}$	$\bar{x}, x, \frac{1}{2}$
6	<i>l</i>	<i>m m 2</i>	$x, 2x, 0$	$2\bar{x}, \bar{x}, 0$	$x, \bar{x}, 0$	$\bar{x}, 2\bar{x}, 0$	$2x, x, 0$	$\bar{x}, x, 0$
6	<i>k</i>	<i>m 2 m</i>	$x, 0, \frac{1}{2}$	$0, x, \frac{1}{2}$	$\bar{x}, \bar{x}, \frac{1}{2}$	$\bar{x}, 0, \frac{1}{2}$	$0, \bar{x}, \frac{1}{2}$	$x, x, \frac{1}{2}$
6	<i>j</i>	<i>m 2 m</i>	$x, 0, 0$	$0, x, 0$	$\bar{x}, \bar{x}, 0$	$\bar{x}, 0, 0$	$0, \bar{x}, 0$	$x, x, 0$
6	<i>i</i>	<i>2 m m</i>	$\frac{1}{2}, 0, z$	$0, \frac{1}{2}, z$	$\frac{1}{2}, \frac{1}{2}, z$	$0, \frac{1}{2}, \bar{z}$	$\frac{1}{2}, 0, \bar{z}$	$\frac{1}{2}, \frac{1}{2}, \bar{z}$
4	<i>h</i>	<i>3 m .</i>	$\frac{1}{3}, \frac{2}{3}, z$	$\frac{2}{3}, \frac{1}{3}, z$	$\frac{2}{3}, \frac{1}{3}, \bar{z}$	$\frac{1}{3}, \frac{2}{3}, \bar{z}$		
3	<i>g</i>	<i>m m m</i>	$\frac{1}{2}, 0, \frac{1}{2}$	$0, \frac{1}{2}, \frac{1}{2}$	$\frac{1}{2}, \frac{1}{2}, \frac{1}{2}$			
3	<i>f</i>	<i>m m m</i>	$\frac{1}{2}, 0, 0$	$0, \frac{1}{2}, 0$	$\frac{1}{2}, \frac{1}{2}, 0$			
2	<i>e</i>	<i>6 m m</i>	$0, 0, z$	$0, 0, \bar{z}$				
2	<i>d</i>	$\bar{6} m 2$	$\frac{1}{3}, \frac{2}{3}, \frac{1}{2}$	$\frac{2}{3}, \frac{1}{3}, \frac{1}{2}$				
2	<i>c</i>	$\bar{6} m 2$	$\frac{1}{3}, \frac{2}{3}, 0$	$\frac{2}{3}, \frac{1}{3}, 0$				
1	<i>b</i>	<i>6/m m m</i>	$0, 0, \frac{1}{2}$					
1	<i>a</i>	<i>6/m m m</i>	$0, 0, 0$					

Symmetry of special projections

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

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

Along [210] *p2mm*
 $\mathbf{a}' = \frac{1}{2}\mathbf{b}$ $\mathbf{b}' = \mathbf{c}$
 Origin at x, $\frac{1}{2}x, 0$

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