

$P\bar{3}1m$

D_{3d}^1

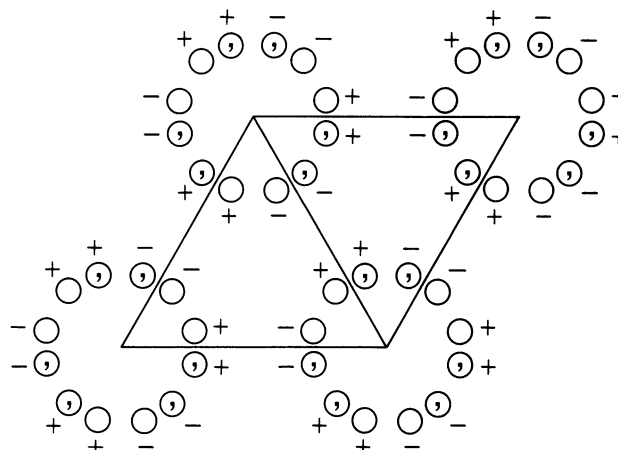
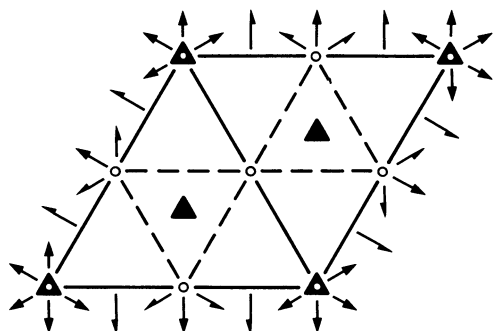
$\bar{3}1m$

Trigonal

No. 162

$P\bar{3}12/m$

Patterson symmetry $P\bar{3}1m$



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

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

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

Symmetry operations

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

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	l	1	(1) x, y, z (4) $\bar{y}, \bar{x}, \bar{z}$ (7) $\bar{x}, \bar{y}, \bar{z}$ (10) y, x, z	(2) $\bar{y}, x - y, z$ (5) $\bar{x} + y, y, \bar{z}$ (8) $y, \bar{x} + y, \bar{z}$ (11) $x - y, \bar{y}, z$	(3) $\bar{x} + y, \bar{x}, z$ (6) $x, x - y, \bar{z}$ (9) $x - y, x, \bar{z}$ (12) $\bar{x}, \bar{x} + y, z$	no conditions		
					Special: no extra conditions			
6	k	$\dots m$	$x, 0, z$	$0, x, z$	\bar{x}, \bar{x}, z	$0, \bar{x}, \bar{z}$	$\bar{x}, 0, \bar{z}$	x, x, \bar{z}
6	j	$\dots 2$	$x, \bar{x}, \frac{1}{2}$	$x, 2x, \frac{1}{2}$	$2\bar{x}, \bar{x}, \frac{1}{2}$	$\bar{x}, x, \frac{1}{2}$	$\bar{x}, 2\bar{x}, \frac{1}{2}$	$2x, x, \frac{1}{2}$
6	i	$\dots 2$	$x, \bar{x}, 0$	$x, 2x, 0$	$2\bar{x}, \bar{x}, 0$	$\bar{x}, x, 0$	$\bar{x}, 2\bar{x}, 0$	$2x, x, 0$
4	h	$3\dots$	$\frac{1}{3}, \frac{2}{3}, z$	$\frac{1}{3}, \frac{2}{3}, \bar{z}$	$\frac{2}{3}, \frac{1}{3}, \bar{z}$	$\frac{2}{3}, \frac{1}{3}, z$		
3	g	$\dots 2/m$	$\frac{1}{2}, 0, \frac{1}{2}$	$0, \frac{1}{2}, \frac{1}{2}$	$\frac{1}{2}, \frac{1}{2}, \frac{1}{2}$			
3	f	$\dots 2/m$	$\frac{1}{2}, 0, 0$	$0, \frac{1}{2}, 0$	$\frac{1}{2}, \frac{1}{2}, 0$			
2	e	$3.m$	$0, 0, z$	$0, 0, \bar{z}$				
2	d	3.2	$\frac{1}{3}, \frac{2}{3}, \frac{1}{2}$	$\frac{2}{3}, \frac{1}{3}, \frac{1}{2}$				
2	c	3.2	$\frac{1}{3}, \frac{2}{3}, 0$	$\frac{2}{3}, \frac{1}{3}, 0$				
1	b	$\bar{3}.m$	$0, 0, \frac{1}{2}$					
1	a	$\bar{3}.m$	$0, 0, 0$					

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] $p2$
 $\mathbf{a}' = \frac{1}{2}\mathbf{b}$ $\mathbf{b}' = \mathbf{c}$
 Origin at $x, \frac{1}{2}x, 0$

Maximal non-isomorphic subgroups

I	[2] $P\bar{3}1m$ (157)	1; 2; 3; 10; 11; 12
	[2] $P\bar{3}12$ (149)	1; 2; 3; 4; 5; 6
	[2] $P\bar{3}11$ ($P\bar{3}$, 147)	1; 2; 3; 7; 8; 9
	{ [3] $P112/m$ ($C2/m$, 12)	1; 4; 7; 10
	{ [3] $P112/m$ ($C2/m$, 12)	1; 5; 7; 11
	{ [3] $P112/m$ ($C2/m$, 12)	1; 6; 7; 12

IIa none

IIb [2] $P\bar{3}1c$ ($\mathbf{c}' = 2\mathbf{c}$) (163); [3] $H\bar{3}1m$ ($\mathbf{a}' = 3\mathbf{a}, \mathbf{b}' = 3\mathbf{b}$) ($P\bar{3}m1$, 164); [3] $R\bar{3}m$ ($\mathbf{a}' = \mathbf{a} - \mathbf{b}, \mathbf{b}' = \mathbf{a} + 2\mathbf{b}, \mathbf{c}' = 3\mathbf{c}$) (166);
 [3] $R\bar{3}m$ ($\mathbf{a}' = 2\mathbf{a} + \mathbf{b}, \mathbf{b}' = -\mathbf{a} + \mathbf{b}, \mathbf{c}' = 3\mathbf{c}$) (166)

Maximal isomorphic subgroups of lowest index

IIc [2] $P\bar{3}1m$ ($\mathbf{c}' = 2\mathbf{c}$) (162); [4] $P\bar{3}1m$ ($\mathbf{a}' = 2\mathbf{a}, \mathbf{b}' = 2\mathbf{b}$) (162)

Minimal non-isomorphic supergroups

I [2] $P6/mmm$ (191); [2] $P6_3/mcm$ (193)
II [3] $H\bar{3}1m$ ($P\bar{3}m1$, 164)