

$p\bar{3}1m$

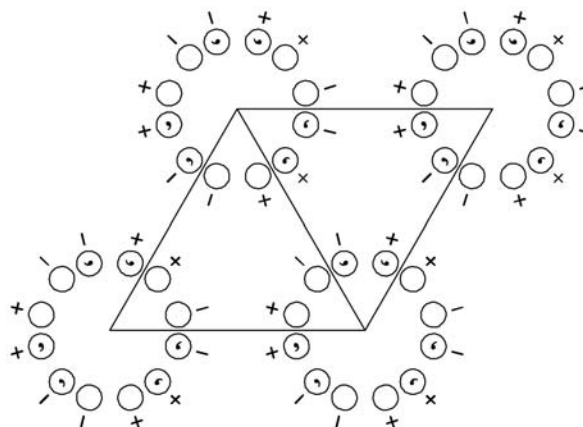
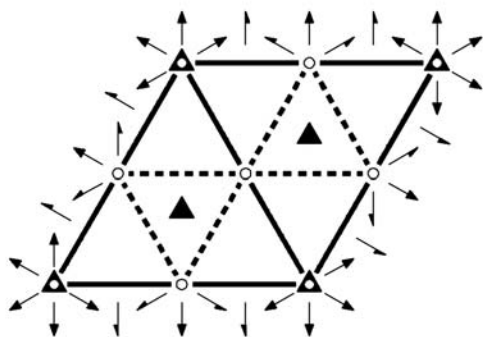
$\bar{3}1m$

Trigonal/Hexagonal

No. 71

$p\bar{3}12/m$

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



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

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

Symmetry operations

- | | | |
|--|---|--|
| (1) 1
(1 0,0,0) | (2) 3^+ 0,0,z
(3_z 0,0,0) | (3) 3^- 0,0,z
(3_z^{-1} 0,0,0) |
| (4) 2 $x, \bar{x}, 0$
(2_3 0,0,0) | (5) 2 $x, 2x, 0$
(2_2 0,0,0) | (6) 2 $2x, x, 0$
(2_1 0,0,0) |
| (7) $\bar{1}$ 0,0,0
($\bar{1}$ 0,0,0) | (8) $\bar{3}^+$ 0,0,z; 0,0,0
($\bar{3}_z$ 0,0,0) | (9) $\bar{3}^-$ 0,0,z; 0,0,0
($\bar{3}_z^{-1}$ 0,0,0) |
| (10) m x, x, z
(m_3 0,0,0) | (11) m $x, 0, z$
(m_2 0,0,0) | (12) m $0, y, z$
(m_1 0,0,0) |

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

Positions

Multiplicity, Wyckoff letter, Site symmetry		Coordinates				Reflection conditions		
						General:		
12	$h\ 1$	(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	$g\ \dots m$	$x, 0, z$	$0, x, z$	\bar{x}, \bar{x}, z	$0, \bar{x}, \bar{z}$	$\bar{x}, 0, \bar{z}$	x, x, \bar{z}	
6	$f\ \dots 2$	$x, \bar{x}, 0$	$x, 2x, 0$	$2\bar{x}, \bar{x}, 0$	$\bar{x}, x, 0$	$\bar{x}, 2\bar{x}, 0$	$2x, x, 0$	
4	$e\ 3\dots$	$\frac{1}{3}, \frac{2}{3}, z$	$\frac{1}{3}, \frac{2}{3}, \bar{z}$	$\frac{2}{3}, \frac{1}{3}, \bar{z}$	$\frac{2}{3}, \frac{1}{3}, z$			
3	$d\ \dots 2/m$	$\frac{1}{2}, 0, 0$	$0, \frac{1}{2}, 0$	$\frac{1}{2}, \frac{1}{2}, 0$				
2	$c\ 3\dots m$	$0, 0, z$	$0, 0, \bar{z}$					
2	$b\ 3\dots 2$	$\frac{1}{3}, \frac{2}{3}, 0$	$\frac{2}{3}, \frac{1}{3}, 0$					
1	$a\ \bar{3}\dots m$	$0, 0, 0$						

Symmetry of special projections

Along [001] $p6mm$

$\mathbf{a}' = \mathbf{a}$ $\mathbf{b}' = \mathbf{b}$

Origin at $0, 0, z$

Along [100] $\not\neq 2mm$

$\mathbf{a}' = \frac{1}{2}(\mathbf{a} + 2\mathbf{b})$

Origin at $x, 0, 0$

Along [210] $\not\neq 211$

$\mathbf{a}' = \frac{1}{2}\mathbf{b}$

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

Maximal non-isotypic subgroups

I	[2] $p\bar{3}1m$ (70)	1; 2; 3; 10; 11; 12
	[2] $p\bar{3}12$ (67)	1; 2; 3; 4; 5; 6
	[2] $p\bar{3}11$ ($p\bar{3}$, 66)	1; 2; 3; 7; 8; 9
	[3] $p112/m$ ($c2/m11$, 18)	1; 4; 7; 10
	[3] $p112/m$ ($c2/m11$, 18)	1; 5; 7; 11
	[3] $p112/m$ ($c2/m11$, 18)	1; 6; 7; 12

IIa none

IIb [3] $h\bar{3}1m$ ($\mathbf{a}' = 3\mathbf{a}, \mathbf{b}' = 3\mathbf{b}$) ($p\bar{3}m1$, 72)

Maximal isotypic subgroups of lowest index

IIc [4] $p\bar{3}1m$ ($\mathbf{a}' = 2\mathbf{a}, \mathbf{b}' = 2\mathbf{b}$) (71)

Minimal non-isotypic supergroups

I [2] $p6/mmm$ (80)

II [2] $h\bar{3}1m$ ($p\bar{3}m1$, 72)