

$\bar{3}1m$

$\bar{3}1m$

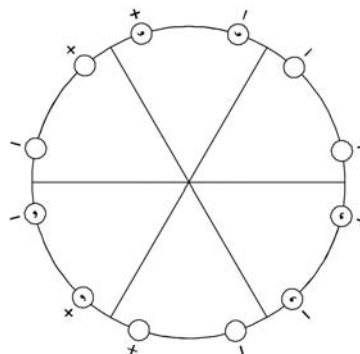
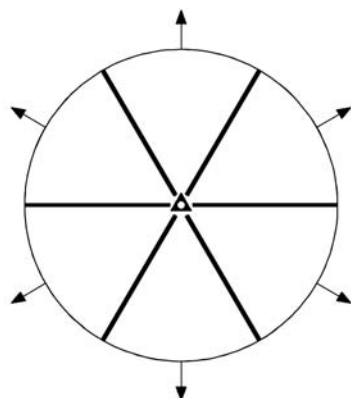
Trigonal

No. 51

$\bar{3}12/m$

Patterson symmetry $\bar{3}1m$

FIRST SETTING



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

Asymmetric unit $0 \leq x; 0 \leq y; 0 \leq z \leq \frac{1}{2}; y \leq x$

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

Positions

Multiplicity, Wyckoff letter, Site symmetry	Coordinates							Reflection conditions
12 <i>g</i> 1	(1) x, y, z	(2) $\bar{y}, x - y, z$	(3) $\bar{x} + y, \bar{x}, z$					General: no conditions
	(4) $\bar{y}, \bar{x}, \bar{z}$	(5) $\bar{x} + y, y, \bar{z}$	(6) $x, x - y, \bar{z}$					
	(7) $\bar{x}, \bar{y}, \bar{z}$	(8) $y, \bar{x} + y, \bar{z}$	(9) $x - y, x, \bar{z}$					
	(10) y, x, z	(11) $x - y, \bar{y}, z$	(12) $\bar{x}, \bar{x} + y, z$					Special: no extra conditions
6 <i>f</i> $\dots m$	$x, 0, z$	$0, x, z$	\bar{x}, \bar{x}, z	$0, \bar{x}, \bar{z}$	$\bar{x}, 0, \bar{z}$	x, x, \bar{z}		
6 <i>e</i> $\dots 2$	$x, \bar{x}, \frac{1}{2}$	$x, 2x, \frac{1}{2}$	$2\bar{x}, \bar{x}, \frac{1}{2}$	$\bar{x}, x, \frac{1}{2}$	$\bar{x}, 2\bar{x}, \frac{1}{2}$	$2x, x, \frac{1}{2}$		
6 <i>d</i> $\dots 2$	$x, \bar{x}, 0$	$x, 2x, 0$	$2\bar{x}, \bar{x}, 0$	$\bar{x}, x, 0$	$\bar{x}, 2\bar{x}, 0$	$2x, x, 0$		
2 <i>c</i> $3 \dots m$	$0, 0, z$	$0, 0, \bar{z}$						
1 <i>b</i> $\bar{3} \dots m$	$0, 0, \frac{1}{2}$							
1 <i>a</i> $\bar{3} \dots m$	$0, 0, 0$							

Symmetry of special projections

Along [001] $6mm$

Along [100] $\bar{3}2mm$

Along [210] $\bar{3}211$

Origin at $0, 0, z$

$\mathbf{a}' = \mathbf{c}$
Origin at $x, 0, 0$

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

Maximal non-isotypic non-enantiomorphic subgroups

I	$[2]\bar{3}1m$ ($\bar{3}1m$, 49)	1; 2; 3; 10; 11; 12
	$[2]\bar{3}12$ (46)	1; 2; 3; 4; 5; 6
	$[2]\bar{3}11$ ($\bar{3}$, 45)	1; 2; 3; 7; 8; 9
	$[3]\bar{1}12/m$ ($\bar{2}/m11$, 6)	1; 4; 7; 10
	$[3]\bar{1}12/m$ ($\bar{2}/m11$, 6)	1; 5; 7; 11
	$[3]\bar{1}12/m$ ($\bar{2}/m11$, 6)	1; 6; 7; 12

IIa none

IIb $[2]\bar{3}1c$ ($c' = 2c$) (52)

Maximal isotypic subgroups and enantiomorphic subgroups of lowest index

IIc $[2]\bar{3}1m$ ($c' = 2c$) (51)

Minimal non-isotypic non-enantiomorphic supergroups

I $[2]\bar{6}/mmm$ (73); $[2]\bar{6}_3/mmc$ (75)

II none

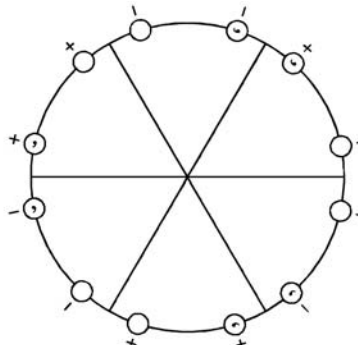
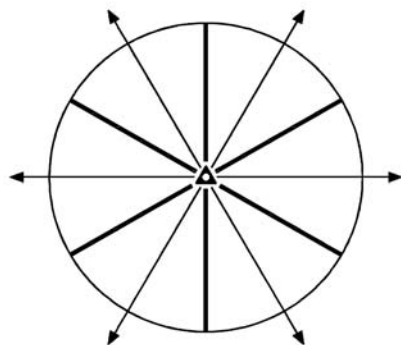
$\bar{3}m1$ $\bar{3}m1$

Trigonal

No. 51

 $\bar{3}2/m1$ Patterson symmetry $\bar{3}m1$

SECOND SETTING

**Origin** at centre ($\bar{3}m1$)**Asymmetric unit** $0 \leq x; 0 \leq y; 0 \leq z \leq 1; y \leq x/2$ **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,x,0
(2_{xy} 0,0,0) | (5) 2 x,0,0
(2_x 0,0,0) | (6) 2 0,y,0
(2_y 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, \bar{x} ,z
(m_{xy} 0,0,0) | (11) m x,2x,z
(m_x 0,0,0) | (12) m 2x,x,z
(m_y 0,0,0) |

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

Positions

Multiplicity, Wyckoff letter, Site symmetry		Coordinates						Reflection conditions
12	g 1	(1) x, y, z	(2) $\bar{y}, x - y, z$	(3) $\bar{x} + y, \bar{x}, z$				General: no conditions
		(4) y, x, \bar{z}	(5) $x - y, \bar{y}, \bar{z}$	(6) $\bar{x}, \bar{x} + y, \bar{z}$				
		(7) $\bar{x}, \bar{y}, \bar{z}$	(8) $y, \bar{x} + y, \bar{z}$	(9) $x - y, x, \bar{z}$				
		(10) \bar{y}, \bar{x}, z	(11) $\bar{x} + y, y, z$	(12) $x, x - y, z$				Special: no extra conditions
6	f . m .	x, \bar{x}, z	$x, 2x, z$	$2\bar{x}, \bar{x}, z$	\bar{x}, x, \bar{z}	$2x, x, \bar{z}$	$\bar{x}, 2\bar{x}, \bar{z}$	
6	e . 2 .	$x, 0, \frac{1}{2}$	$0, x, \frac{1}{2}$	$\bar{x}, \bar{x}, \frac{1}{2}$	$\bar{x}, 0, \frac{1}{2}$	$0, \bar{x}, \frac{1}{2}$	$x, x, \frac{1}{2}$	
6	d . 2 .	$x, 0, 0$	$0, x, 0$	$\bar{x}, \bar{x}, 0$	$\bar{x}, 0, 0$	$0, \bar{x}, 0$	$x, x, 0$	
2	c 3 m .	$0, 0, z$	$0, 0, \bar{z}$					
1	b $\bar{3}m$.	$0, 0, \frac{1}{2}$						
1	a $\bar{3}m$.	$0, 0, 0$						

Symmetry of special projections

Along [001] $6mm$

Along [100] $\bar{3}211$

Along [210] $\bar{3}2mm$

Origin at $0, 0, z$

$\mathbf{a}' = \mathbf{c}$
Origin at $x, 0, 0$

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

Maximal non-isotypic non-enantiomorphic subgroups

I	$[2]\bar{3}m1$ (49)	1; 2; 3; 10; 11; 12
	$[2]\bar{3}21$ ($\bar{3}12, 46$)	1; 2; 3; 4; 5; 6
	$[2]\bar{3}11$ ($\bar{3}, 45$)	1; 2; 3; 7; 8; 9
	$[3]\bar{3}12/m1$ ($\bar{3}2/m11, 6$)	1; 4; 7; 10
	$[3]\bar{3}12/m1$ ($\bar{3}2/m11, 6$)	1; 5; 7; 11
	$[3]\bar{3}12/m1$ ($\bar{3}2/m11, 6$)	1; 6; 7; 12

IIa none

IIb $[2]\bar{3}c1$ ($\mathbf{c}' = 2\mathbf{c}$) ($\bar{3}1c, 52$)

Maximal isotypic subgroups and enantiomorphic subgroups of lowest index

IIc $[2]\bar{3}m1$ ($\mathbf{c}' = 2\mathbf{c}$) ($\bar{3}1m, 51$)

Minimal non-isotypic non-enantiomorphic supergroups

I $[2]\bar{6}/mmm$ (73); $[2]\bar{6}_3/mmc$ (75)

II none