

$\bar{3}m1$

$3m1$

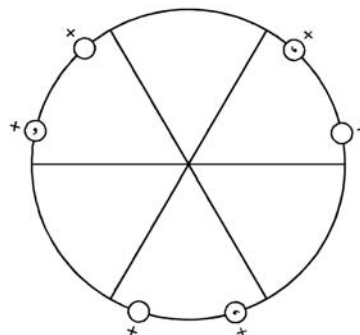
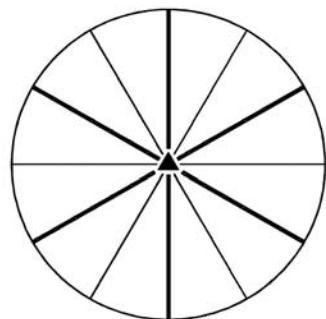
Trigonal

No. 49

$\bar{3}m1$

Patterson symmetry $\bar{3}m1$

FIRST SETTING



Origin on $3m1$

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

Symmetry operations

- | | | |
|---------------------|-----------------|-----------------|
| (1) 1 | (2) $3^+ 0,0,z$ | (3) $3^- 0,0,z$ |
| (4) $m x,\bar{x},z$ | (5) $m x,2x,z$ | (6) $m 2x,x,z$ |

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

Positions

	Multiplicity, Wyckoff letter, Site symmetry	Coordinates			Reflection conditions
6	c 1	(1) x, y, z (4) \bar{y}, \bar{x}, z	(2) $\bar{y}, x - y, z$ (5) $\bar{x} + y, y, z$	(3) $\bar{x} + y, \bar{x}, z$ (6) $x, x - y, z$	General: no conditions Special: no extra conditions
3	b . m .	x, \bar{x}, z	$x, 2x, z$	$2\bar{x}, \bar{x}, z$	
1	a 3 m .	$0, 0, z$			

Symmetry of special projections

Along [001] $3m$	Along [100] $\bar{3}1$	Along [210] $\bar{3}11m$
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	$[2]\bar{3}111$ ($\bar{3}3, 42$)	1; 2; 3
	$[3]\bar{3}1m1$ ($\bar{3}m11, 4$)	1; 4
	$[3]\bar{3}1m1$ ($\bar{3}m11, 4$)	1; 5
	$[3]\bar{3}1m1$ ($\bar{3}m11, 4$)	1; 6

IIa none

IIb $[2]\bar{3}c1$ ($c' = 2c$) (50)

Maximal isotypic subgroups and enantiomorphic subgroups of lowest index

IIc $[2]\bar{3}m1$ ($c' = 2c$) (49)

Minimal non-isotypic non-enantiomorphic supergroups

I $[2]\bar{3}1m$ (51); $[2]\bar{3}6mm$ (68); $[2]\bar{3}6_3mc$ (70); $[2]\bar{3}6m2$ (71)

II none

$\bar{3}1m$

$31m$

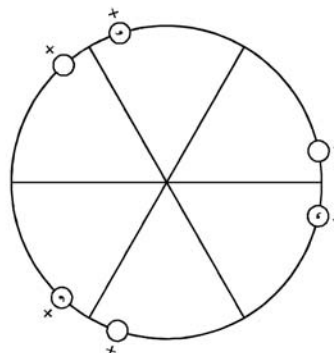
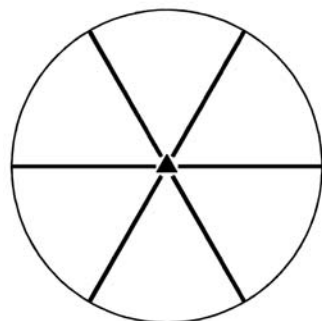
Trigonal

No. 49

$\bar{3}1m$

Patterson symmetry $\bar{3}1m$

SECOND SETTING



Origin on $31m$

Asymmetric unit $0 \leq x; 0 \leq y; 0 \leq z \leq 1; y \leq x$

Symmetry operations

- | | | |
|---------------|-----------------|-----------------|
| (1) 1 | (2) $3^+ 0,0,z$ | (3) $3^- 0,0,z$ |
| (4) $m x,x,z$ | (5) $m x,0,z$ | (6) $m 0,y,z$ |

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

Positions

Multiplicity, Wyckoff letter, Site symmetry		Coordinates			Reflection conditions
6	c 1	(1) x, y, z (4) y, x, z	(2) $\bar{y}, x - y, z$ (5) $x - y, \bar{y}, z$	(3) $\bar{x} + y, \bar{x}, z$ (6) $\bar{x}, \bar{x} + y, z$	General: no conditions Special: no extra conditions
3	b $\dots m$	$x, 0, z$	$0, x, z$	\bar{x}, \bar{x}, z	
1	a $3 \dots m$	$0, 0, z$			

Symmetry of special projections

Along [001] $3m$	Along [100] $\bar{3}11m$	Along [210] $\bar{3}1$
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	$[2]\bar{3}11$ ($\bar{3}, 42$)	1; 2; 3
	$[3]\bar{3}11m$ ($\bar{3}m11, 4$)	1; 4
	$[3]\bar{3}11m$ ($\bar{3}m11, 4$)	1; 5
	$[3]\bar{3}11m$ ($\bar{3}m11, 4$)	1; 6

IIa none

IIb $[2]\bar{3}1c$ ($\mathbf{c}' = 2\mathbf{c}$) ($\bar{3}c1, 50$)

Maximal isotypic subgroups and enantiomorphic subgroups of lowest index

IIc $[2]\bar{3}1m$ ($\mathbf{c}' = 2\mathbf{c}$) ($\bar{3}m1, 49$)

Minimal non-isotypic non-enantiomorphic supergroups

I $[2]\bar{3}1m$ (51); $[2]\bar{6}mm$ (68); $[2]\bar{6}_3mc$ (70); $[2]\bar{6}m2$ (71)

II none