

$\bar{3}c1$

$3m1$

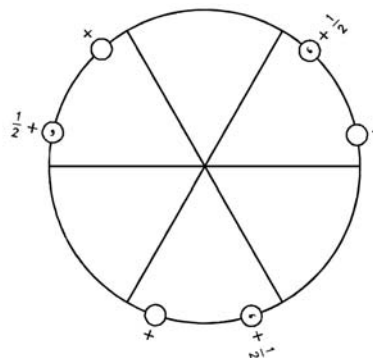
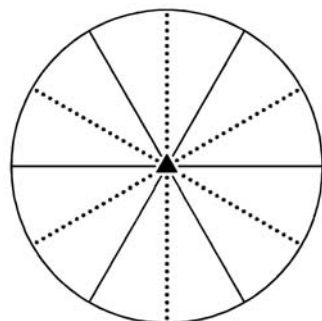
Trigonal

No. 50

$\bar{3}c1$

Patterson symmetry $\bar{3}m1$

FIRST SETTING



Origin on $3c1$

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

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) c x, \bar{x} ,z
(m_{xy} 0,0, $\frac{1}{2}$) | (5) c x,2x,z
(m_x 0,0, $\frac{1}{2}$) | (6) c 2x,x,z
(m_y 0,0, $\frac{1}{2}$) |

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

Positions

Multiplicity, Wyckoff letter, Site symmetry	Coordinates			Reflection conditions
				General:
6 <i>b</i> 1	(1) x, y, z (4) $\bar{y}, \bar{x}, z + \frac{1}{2}$	(2) $\bar{y}, x - y, z$ (5) $\bar{x} + y, y, z + \frac{1}{2}$	(3) $\bar{x} + y, \bar{x}, z$ (6) $x, x - y, z + \frac{1}{2}$	$l : l = 2n$
2 <i>a</i> 3..	0, 0, z	0, 0, $z + \frac{1}{2}$		Special: no extra conditions

Symmetry of special projections

Along [001] $3m$	Along [100] $\bar{3}1$	Along [210] $\bar{3}11g$
Origin at 0, 0, z	$\mathbf{a}' = \frac{1}{2}\mathbf{c}$ 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
	$[3]\bar{1}c1 (\bar{1}c11, 5)$	1; 4
	$[3]\bar{1}c1 (\bar{1}c11, 5)$	1; 5
	$[3]\bar{1}c1 (\bar{1}c11, 5)$	1; 6

IIa none

IIb none

Maximal isotypic subgroups and enantiomorphic subgroups of lowest index

IIc $[3]\bar{3}c1 (\mathbf{c}' = 3\mathbf{c}) (50)$

Minimal non-isotypic non-enantiomorphic supergroups

I $[2]\bar{3}1c (52)$; $[2]\bar{6}cc (69)$; $[2]\bar{6}_3mc (70)$; $[2]\bar{6}c2 (72)$

II $[2]\bar{3}m1 (\mathbf{c}' = \frac{1}{2}\mathbf{c}) (49)$

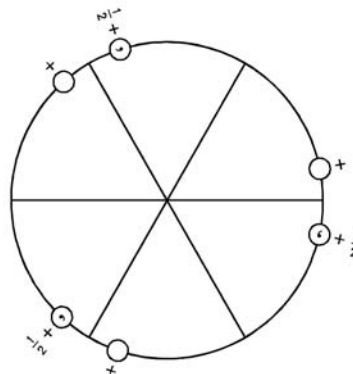
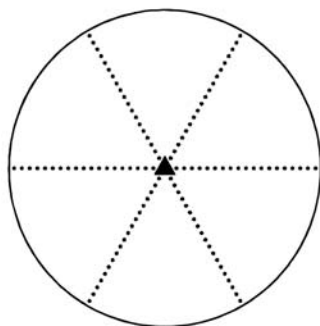
$\bar{3}1c$ $31m$

Trigonal

No. 50

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

SECOND SETTING

Origin on $31c$ Asymmetric unit $0 \leq x; 0 \leq y; 0 \leq z \leq \frac{1}{2}$

Symmetry operations

- | | | |
|--|--|--|
| (1) 1
(1 0,0,0) | (2) 3^+ 0,0,z
(3_2 0,0,0) | (3) 3^- 0,0,z
(3_2^{-1} 0,0,0) |
| (4) c x,x,z
(m_3 0,0, $\frac{1}{2}$) | (5) c x,0,z
(m_2 0,0, $\frac{1}{2}$) | (6) c 0,y,z
(m_1 0,0, $\frac{1}{2}$) |

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

Positions

Multiplicity, Wyckoff letter, Site symmetry	Coordinates			Reflection conditions
				General:
6 <i>b</i> 1	(1) x, y, z (4) $y, x, z + \frac{1}{2}$	(2) $\bar{y}, x - y, z$ (5) $x - y, \bar{y}, z + \frac{1}{2}$	(3) $\bar{x} + y, \bar{x}, z$ (6) $\bar{x}, \bar{x} + y, z + \frac{1}{2}$	$l : l = 2n$
2 <i>a</i> 3..	0, 0, z	0, 0, $z + \frac{1}{2}$		Special: no extra conditions

Symmetry of special projections

Along [001] $3m$	Along [100] $\bar{3}11g$	Along [210] $\bar{3}1$
Origin at 0, 0, z	$\mathbf{a}' = \mathbf{c}$ Origin at $x, 0, 0$	$\mathbf{a}' = \frac{1}{2}\mathbf{c}$ Origin at $x, \frac{1}{2}x, 0$

Maximal non-isotypic non-enantiomorphic subgroups

I	$[2]\bar{3}11c$ ($\bar{3}3, 42$)	1; 2; 3
	$[3]\bar{3}11c$ ($\bar{3}c11, 5$)	1; 4
	$[3]\bar{3}11c$ ($\bar{3}c11, 5$)	1; 5
	$[3]\bar{3}11c$ ($\bar{3}c11, 5$)	1; 6

IIa none

IIb none

Maximal isotypic subgroups and enantiomorphic subgroups of lowest index

IIc $[3]\bar{3}11c$ ($\mathbf{c}' = 3\mathbf{c}$) ($\bar{3}3c1, 50$)

Minimal non-isotypic non-enantiomorphic supergroups

I	$[2]\bar{3}11c$ (52); $[2]\bar{3}6cc$ (69); $[2]\bar{3}6_3mc$ (70); $[2]\bar{3}6c2$ (72)
II	$[2]\bar{3}3m1$ ($\mathbf{c}' = \frac{1}{2}\mathbf{c}$) (49)