

$\bar{3}1c$

$\bar{3}1m$

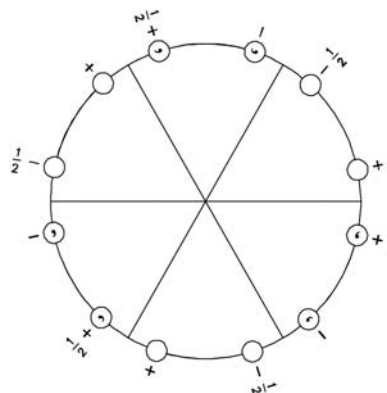
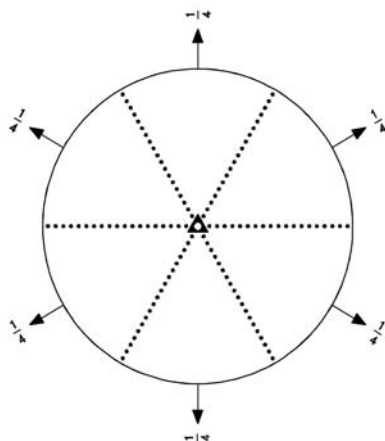
Trigonal

No. 52

$\bar{3}12/c$

Patterson symmetry $\bar{3}1m$

FIRST SETTING



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

Asymmetric unit $0 \leq x; 0 \leq y; 0 \leq z \leq \frac{1}{4}$

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 $x, \bar{x}, \frac{1}{4}$
(2_3 0,0, $\frac{1}{2}$) | (5) 2 $x, 2x, \frac{1}{4}$
(2_2 0,0, $\frac{1}{2}$) | (6) 2 $2x, x, \frac{1}{4}$
(2_1 0,0, $\frac{1}{2}$) |
| (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) c x, x, z
(m_3 0,0, $\frac{1}{2}$) | (11) c $x, 0, z$
(m_2 0,0, $\frac{1}{2}$) | (12) c $0, y, z$
(m_1 0,0, $\frac{1}{2}$) |

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

Positions

Multiplicity, Wyckoff letter, Site symmetry		Coordinates						Reflection conditions
								General:
12	e 1	(1) x, y, z	(2) $\bar{y}, x - y, z$	(3) $\bar{x} + y, \bar{x}, z$	(4) $\bar{y}, \bar{x}, \bar{z} + \frac{1}{2}$	(5) $\bar{x} + y, y, \bar{z} + \frac{1}{2}$	(6) $x, x - y, \bar{z} + \frac{1}{2}$	$l : l = 2n$
		(7) $\bar{x}, \bar{y}, \bar{z}$	(8) $y, \bar{x} + y, \bar{z}$	(9) $x - y, x, \bar{z}$	(10) $y, x, z + \frac{1}{2}$	(11) $x - y, \bar{y}, z + \frac{1}{2}$	(12) $\bar{x}, \bar{x} + y, z + \frac{1}{2}$	
								Special: no extra conditions
6	d ..2	$x, \bar{x}, \frac{1}{4}$	$x, 2x, \frac{1}{4}$	$2\bar{x}, \bar{x}, \frac{1}{4}$	$\bar{x}, x, \frac{3}{4}$	$\bar{x}, 2\bar{x}, \frac{3}{4}$	$2x, x, \frac{3}{4}$	
4	c 3..	$0, 0, z$	$0, 0, \bar{z} + \frac{1}{2}$	$0, 0, \bar{z}$	$0, 0, z + \frac{1}{2}$			
2	b $\bar{3}$..	$0, 0, 0$	$0, 0, \frac{1}{2}$					
2	a 3.2	$0, 0, \frac{1}{4}$	$0, 0, \frac{3}{4}$					

Symmetry of special projections

Along [001] $6mm$

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

Along [210] $\bar{2}11$

Origin at $0, 0, z$

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

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

Origin at $x, 0, 0$

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

Maximal non-isotypic non-enantiomorphic subgroups

I	$[2]\bar{3}1c$ ($\bar{3}c1, 50$)	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
	$[3]\bar{1}12/c$ ($\bar{2}/c11, 7$)	1; 4; 7; 10
	$[3]\bar{1}12/c$ ($\bar{2}/c11, 7$)	1; 5; 7; 11
	$[3]\bar{1}12/c$ ($\bar{2}/c11, 7$)	1; 6; 7; 12

IIa none

IIb none

Maximal isotypic subgroups and enantiomorphic subgroups of lowest index

IIc $[3]\bar{3}1c$ ($\mathbf{c}' = 3\mathbf{c}$) (52)

Minimal non-isotypic non-enantiomorphic supergroups

I $[2]\bar{6}/mcc$ (74); $[2]\bar{6}_3/mmc$ (75)

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

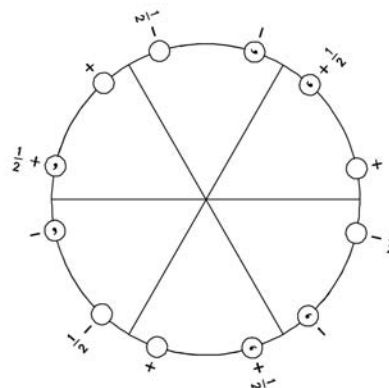
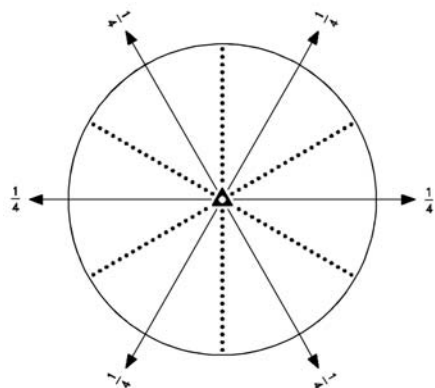
$\bar{3}c1$ $\bar{3}m1$

Trigonal

No. 52

 $\bar{3}2/c1$ Patterson symmetry $\bar{3}m1$

SECOND SETTING

**Origin** at centre ($\bar{3}$) at $\bar{3}c1$ **Asymmetric unit** $0 \leq x; 0 \leq y; 0 \leq z \leq \frac{1}{4}$ **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 $x, x, \frac{1}{4}$
(2_{xy} 0,0, $\frac{1}{2}$) | (5) 2 $x, 0, \frac{1}{4}$
(2_x 0,0, $\frac{1}{2}$) | (6) 2 $0, y, \frac{1}{4}$
(2_y 0,0, $\frac{1}{2}$) |
| (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) c x, \bar{x}, z
(m_{xy} 0,0, $\frac{1}{2}$) | (11) c $x, 2x, z$
(m_x 0,0, $\frac{1}{2}$) | (12) c $2x, x, z$
(m_y 0,0, $\frac{1}{2}$) |

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

Positions

Multiplicity, Wyckoff letter, Site symmetry		Coordinates						Reflection conditions
								General:
12	e 1	(1) x, y, z	(2) $\bar{y}, x - y, z$	(3) $\bar{x} + y, \bar{x}, z$				$l : l = 2n$
		(4) $y, x, \bar{z} + \frac{1}{2}$	(5) $x - y, \bar{y}, \bar{z} + \frac{1}{2}$	(6) $\bar{x}, \bar{x} + y, \bar{z} + \frac{1}{2}$				
		(7) $\bar{x}, \bar{y}, \bar{z}$	(8) $y, \bar{x} + y, \bar{z}$	(9) $x - y, x, \bar{z}$				
		(10) $\bar{y}, \bar{x}, z + \frac{1}{2}$	(11) $\bar{x} + y, y, z + \frac{1}{2}$	(12) $x, x - y, z + \frac{1}{2}$				
								Special: no extra conditions
6	d .2.	$x, 0, \frac{1}{4}$	$0, x, \frac{1}{4}$	$\bar{x}, \bar{x}, \frac{1}{4}$	$\bar{x}, 0, \frac{3}{4}$	$0, \bar{x}, \frac{3}{4}$	$x, x, \frac{3}{4}$	
4	c 3..	$0, 0, z$	$0, 0, \bar{z} + \frac{1}{2}$	$0, 0, \bar{z}$	$0, 0, z + \frac{1}{2}$			
2	b $\bar{3}$..	$0, 0, 0$	$0, 0, \frac{1}{2}$					
2	a 32.	$0, 0, \frac{1}{4}$	$0, 0, \frac{3}{4}$					

Symmetry of special projections

Along [001] $6mm$

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

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

Origin at $0, 0, z$

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

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

Origin at $x, 0, 0$

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

Maximal non-isotypic non-enantiomorphic subgroups

I	$[2]\bar{3}c1$ (50)	1; 2; 3; 10; 11; 12
	$[2]\bar{3}21$ ($\bar{3}312, 46$)	1; 2; 3; 4; 5; 6
	$[2]\bar{3}11$ ($\bar{3}\bar{3}, 45$)	1; 2; 3; 7; 8; 9
	$[3]\bar{3}12/c1$ ($\bar{3}2/c11, 7$)	1; 4; 7; 10
	$[3]\bar{3}12/c1$ ($\bar{3}2/c11, 7$)	1; 5; 7; 11
	$[3]\bar{3}12/c1$ ($\bar{3}2/c11, 7$)	1; 6; 7; 12

IIa none

IIb none

Maximal isotypic subgroups and enantiomorphic subgroups of lowest index

IIc $[3]\bar{3}c1$ ($\mathbf{c}' = 3\mathbf{c}$) ($\bar{3}31c, 52$)

Minimal non-isotypic non-enantiomorphic supergroups

I $[2]\bar{3}6/mcc$ (74); $[2]\bar{3}6_3/mmc$ (75)

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