

$\bar{3}12$

312

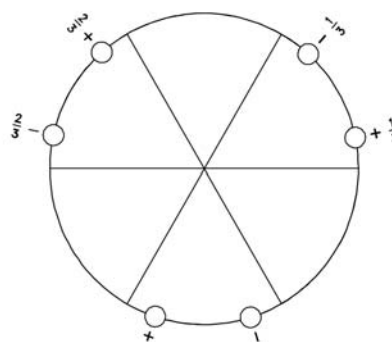
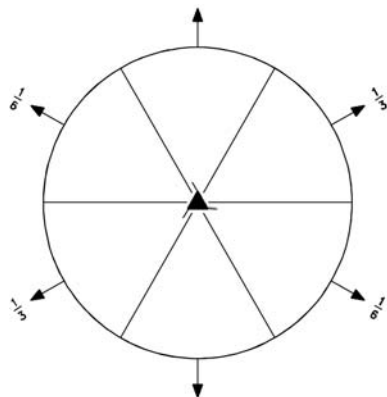
Trigonal

No. 47

$\bar{3}12$

Patterson symmetry $\bar{3}1m$

FIRST SETTING



Origin on $2[210]$ at $3_11(1, 1, 2)$

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

Symmetry operations

- | | | |
|--|---|--|
| (1) 1
(1 0,0,0) | (2) $3^+(\frac{1}{3})$ 0,0,z
(3_z 0,0, $\frac{1}{3}$) | (3) $3^-(\frac{2}{3})$ 0,0,z
(3_z^{-1} 0,0, $\frac{2}{3}$) |
| (4) 2 $x, \bar{x}, \frac{1}{3}$
(2_3 0,0, $\frac{2}{3}$) | (5) 2 $x, 2x, \frac{1}{6}$
(2_2 0,0, $\frac{1}{3}$) | (6) 2 $2x, x, 0$
(2_1 0,0,0) |

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

Positions

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

Symmetry of special projections

Along [001] $3m$	Along [100] $\bar{3}1m1$	Along [210] $\bar{3}211$
Origin at 0, 0, z	$\mathbf{a}' = \mathbf{c}$ Origin at $x, 0, \frac{1}{6}$	$\mathbf{a}' = \mathbf{c}$ Origin at $x, \frac{1}{2}x, 0$

Maximal non-isotypic non-enantiomorphic subgroups

I	[2] $\bar{3}111$ ($\bar{3}1, 43$)	1; 2; 3
	[3] $\bar{1}112$ ($\bar{1}211, 3$)	1; 4
	[3] $\bar{1}112$ ($\bar{1}211, 3$)	1; 5
	[3] $\bar{1}112$ ($\bar{1}211, 3$)	1; 6

IIa none

IIb none

Maximal isotypic subgroups and enantiomorphic subgroups of lowest index

IIc [2] $\bar{3}_212$ ($\mathbf{c}' = 2\mathbf{c}$) (48); [7] $\bar{3}_112$ ($\mathbf{c}' = 7\mathbf{c}$) (47)

Minimal non-isotypic non-enantiomorphic supergroups

I [2] $\bar{6}_122$ (63); [2] $\bar{6}_422$ (66)

II [3] $\bar{3}12$ ($\mathbf{c}' = \frac{1}{3}\mathbf{c}$) (46)

$\bar{3}21$

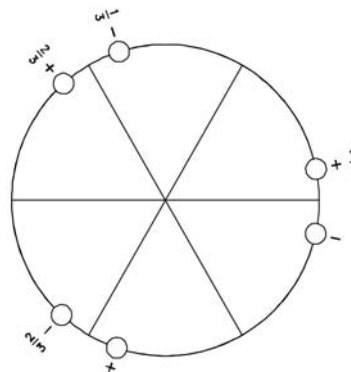
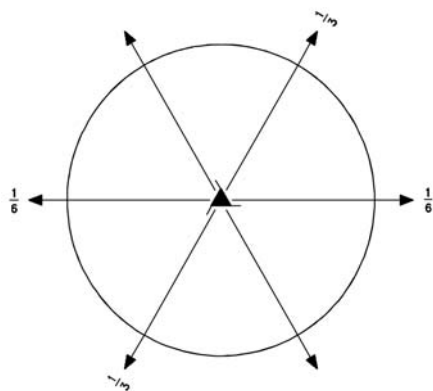
321

Trigonal

No. 47

 $\bar{3}21$ Patterson symmetry $\bar{3}m1$

SECOND SETTING

**Origin** on $2[110]$ at $3_1(1, 1, 2)1$ **Asymmetric unit** $0 \leq x; 0 \leq y; 0 \leq z \leq \frac{1}{2}$ **Symmetry operations**

- | | | |
|-----------------------------------|---|--|
| (1) 1
(1 0,0,0) | (2) $3^+(\frac{1}{3})$ 0,0,z
(3_z 0,0, $\frac{1}{3}$) | (3) $3^-(\frac{2}{3})$ 0,0,z
(3_z^{-1} 0,0, $\frac{2}{3}$) |
| (4) 2 x,x,0
(2_{xy} 0,0,0) | (5) 2 x,0, $\frac{1}{3}$
(2_x 0,0, $\frac{2}{3}$) | (6) 2 0,y, $\frac{1}{6}$
(2_y 0,0, $\frac{1}{3}$) |

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

Positions

Multiplicity,
Wyckoff letter,
Site symmetry

Coordinates

Reflection conditions

General:

$$l : l = 3n$$

Special: no extra conditions

6	<i>c</i>	1	(1) x, y, z	(2) $\bar{y}, x - y, z + \frac{1}{3}$	(3) $\bar{x} + y, \bar{x}, z + \frac{2}{3}$
			(4) y, x, \bar{z}	(5) $x - y, \bar{y}, \bar{z} + \frac{2}{3}$	(6) $\bar{x}, \bar{x} + y, \bar{z} + \frac{1}{3}$

3	<i>b</i>	. 2 .	$x, 0, \frac{5}{6}$	$0, x, \frac{1}{6}$	$\bar{x}, \bar{x}, \frac{1}{2}$
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3	<i>a</i>	. 2 .	$x, 0, \frac{1}{3}$	$0, x, \frac{2}{3}$	$\bar{x}, \bar{x}, 0$
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Symmetry of special projections

Along [001] $3m$

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

Along [210] $\bar{3}1m1$

Origin at $0, 0, z$

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

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

Origin at $x, 0, \frac{1}{3}$

Origin at $x, \frac{1}{2}x, \frac{1}{6}$

Maximal non-isotypic non-enantiomorphic subgroups

I	[2] $\bar{3}11$ ($\bar{3}_1, 43$)	1; 2; 3
	[3] $\bar{1}21$ ($\bar{1}211, 3$)	1; 4
	[3] $\bar{1}21$ ($\bar{1}211, 3$)	1; 5
	[3] $\bar{1}21$ ($\bar{1}211, 3$)	1; 6

IIa none

IIb none

Maximal isotypic subgroups and enantiomorphic subgroups of lowest index

IIc [2] $\bar{3}_221$ ($\mathbf{c}' = 2\mathbf{c}$) ($\bar{3}_212, 48$); [7] $\bar{3}_121$ ($\mathbf{c}' = 7\mathbf{c}$) ($\bar{3}_112, 47$)

Minimal non-isotypic non-enantiomorphic supergroups

I [2] $\bar{6}_122$ (63); [2] $\bar{6}_422$ (66)

II [3] $\bar{3}12$ ($\mathbf{c}' = \frac{1}{3}\mathbf{c}$) (46)