

$\bar{3}212$

312

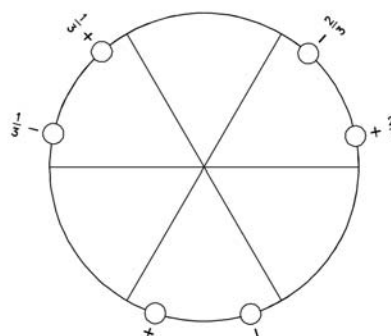
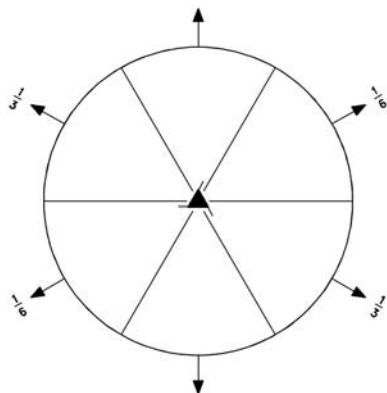
Trigonal

No. 48

$\bar{3}212$

Patterson symmetry $\bar{3}1m$

FIRST SETTING



Origin on $2[210]$ at $3_21(1,1,2)$

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

Symmetry operations

- | | | |
|--|---|--|
| (1) 1
(1 0,0,0) | (2) $3^+(\frac{2}{3})$ 0,0,z
(3_2 0,0, $\frac{2}{3}$) | (3) $3^-(\frac{1}{3})$ 0,0,z
(3_2^{-1} 0,0, $\frac{1}{3}$) |
| (4) 2 $x, \bar{x}, \frac{1}{6}$
(2_3 0,0, $\frac{1}{3}$) | (5) 2 $x, 2x, \frac{1}{3}$
(2_2 0,0, $\frac{2}{3}$) | (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) $\bar{y}, \bar{x}, \bar{z} + \frac{1}{3}$	(2) $\bar{y}, x - y, z + \frac{2}{3}$ (5) $\bar{x} + y, y, \bar{z} + \frac{2}{3}$	(3) $\bar{x} + y, \bar{x}, z + \frac{1}{3}$ (6) $x, x - y, \bar{z}$	General: $l : l = 3n$ Special: no extra conditions
3 <i>b</i> .. 2	$x, \bar{x}, \frac{1}{6}$	$x, 2x, \frac{5}{6}$	$2\bar{x}, \bar{x}, \frac{1}{2}$	
3 <i>a</i> .. 2	$x, \bar{x}, \frac{2}{3}$	$x, 2x, \frac{1}{3}$	$2\bar{x}, \bar{x}, 0$	

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 $x, 0, \frac{1}{3}$	$\mathbf{a}' = \mathbf{c}$ Origin at $x, \frac{1}{2}x, 0$

Maximal non-isotypic non-enantiomorphic subgroups

I	[2] $\bar{3}211$ ($\bar{3}2, 44$)	1; 2; 3
	[3] $\bar{3}112$ ($\bar{3}211, 3$)	1; 4
	[3] $\bar{3}112$ ($\bar{3}211, 3$)	1; 5
	[3] $\bar{3}112$ ($\bar{3}211, 3$)	1; 6

IIa none

IIb none

Maximal isotypic subgroups and enantiomorphic subgroups of lowest index

IIc [2] $\bar{3}12$ ($\mathbf{c}' = 2\mathbf{c}$) (47); [7] $\bar{3}212$ ($\mathbf{c}' = 7\mathbf{c}$) (48)

Minimal non-isotypic non-enantiomorphic supergroups

I [2] $\bar{6}22$ (64); [2] $\bar{6}_522$ (67)

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

$\bar{3}21$

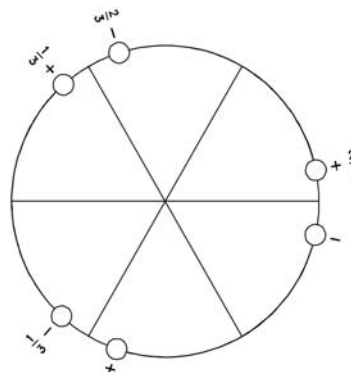
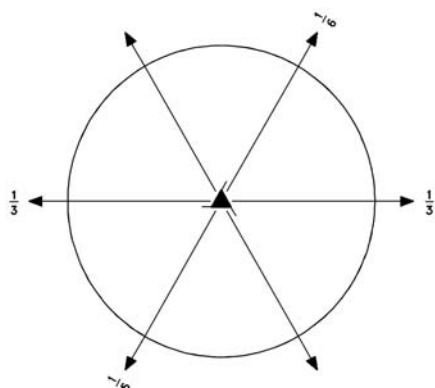
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Trigonal

No. 48

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

SECOND SETTING

**Origin** on $2[110]$ at $3_2(1,1,2)1$ **Asymmetric unit** $0 \leq x; 0 \leq y; 0 \leq z \leq \frac{1}{2}$ **Symmetry operations**

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

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

Symmetry of special projections

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

Maximal non-isotypic non-enantiomorphic subgroups

I	$[2]\bar{3}_211 (\bar{3}_2, 44)$	1; 2; 3
	$[3]\bar{3}121 (\bar{3}211, 3)$	1; 4
	$[3]\bar{3}121 (\bar{3}211, 3)$	1; 5
	$[3]\bar{3}121 (\bar{3}211, 3)$	1; 6

IIa none

IIb none

Maximal isotypic subgroups and enantiomorphic subgroups of lowest index

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

Minimal non-isotypic non-enantiomorphic supergroups

I $[2]\bar{6}_222 (64)$; $[2]\bar{6}_522 (67)$

II $[3]\bar{3}312 (\mathbf{c}' = \frac{1}{3}\mathbf{c}) (46)$