

$\bar{3}12$

312

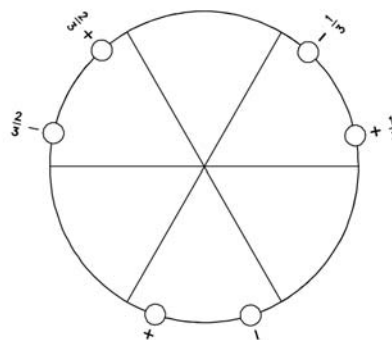
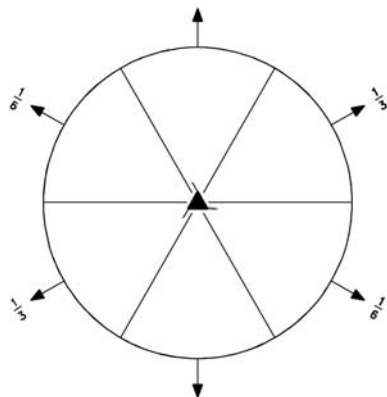
Trigonal

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

**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**

<b>I</b>	$[2]\bar{3}11$ ( $\bar{3}1, 43$ )	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**  $[2]\bar{3}_212$  ( $\mathbf{c}' = 2\mathbf{c}$ ) (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)

$\bar{3}121$ 

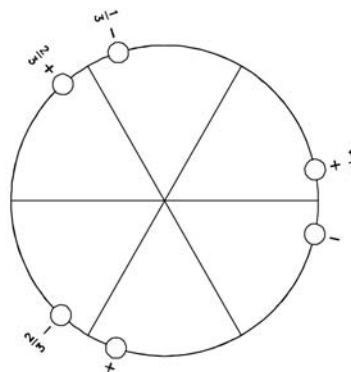
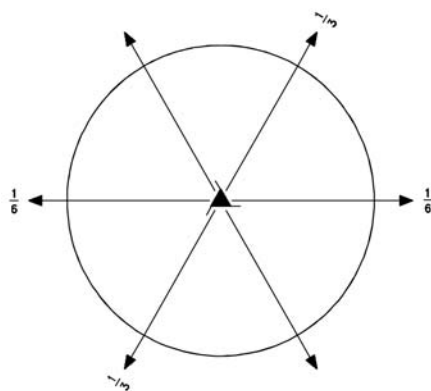
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Trigonal

No. 47

 $\bar{3}121$ 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         | (2) $3^+(\frac{1}{3})$ 0,0,z | (3) $3^-(\frac{2}{3})$ 0,0,z |
| (4) 2 $x,x,0$ | (5) 2 $x,0,\frac{1}{3}$      | (6) 2 $0,y,\frac{1}{6}$      |

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

**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 $x, 0, \frac{1}{3}$	$\mathbf{a}' = \mathbf{c}$ Origin at $x, \frac{1}{2}x, \frac{1}{6}$

**Maximal non-isotypic non-enantiomorphic subgroups**

<b>I</b>	$[2]\bar{3}_111$ ( $\bar{3}_1, 43$ )	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**  $[2]\bar{3}_221$  ( $\mathbf{c}' = 2\mathbf{c}$ ) ( $\bar{3}_212, 48$ );  $[7]\bar{3}_121$  ( $\mathbf{c}' = 7\mathbf{c}$ ) ( $\bar{3}_112, 47$ )

**Minimal non-isotypic non-enantiomorphic supergroups**

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

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