

$\bar{3}12$

312

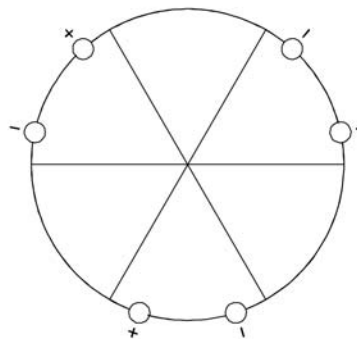
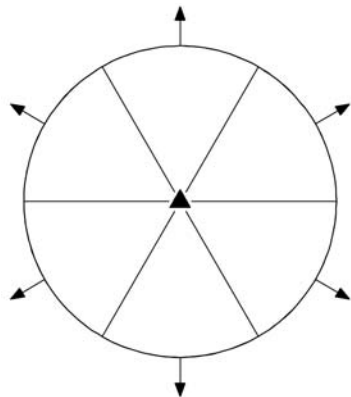
Trigonal

No. 46

$\bar{3}12$

Patterson symmetry $\bar{3}1m$

FIRST SETTING



Origin at 312

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) 2 $x, \bar{x}, 0$
(2_3 0,0,0) | (5) 2 $x, 2x, 0$
(2_2 0,0,0) | (6) 2 $2x, x, 0$
(2_1 0,0,0) |

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

Positions

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

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 $x, 0, 0$	$\mathbf{a}' = \mathbf{c}$ 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
	$[3]\bar{1}112 (\bar{2}111, 3)$	1; 4
	$[3]\bar{1}112 (\bar{2}111, 3)$	1; 5
	$[3]\bar{1}112 (\bar{2}111, 3)$	1; 6

IIa none

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

Maximal isotypic subgroups and enantiomorphic subgroups of lowest index

IIc $[2]\bar{3}12 (\mathbf{c}' = 2\mathbf{c}) (46)$

Minimal non-isotypic non-enantiomorphic supergroups

I	$[2]\bar{3}1m (51)$; $[2]\bar{3}1c (52)$; $[2]\bar{6}22 (62)$; $[2]\bar{6}_322 (65)$; $[2]\bar{6}m2 (71)$; $[2]\bar{6}c2 (72)$
II	none

$\bar{3}21$

321

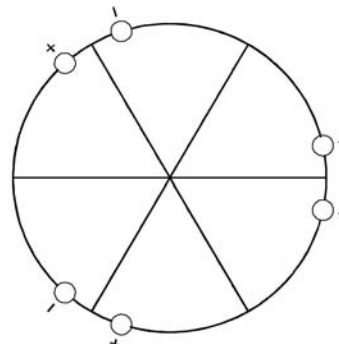
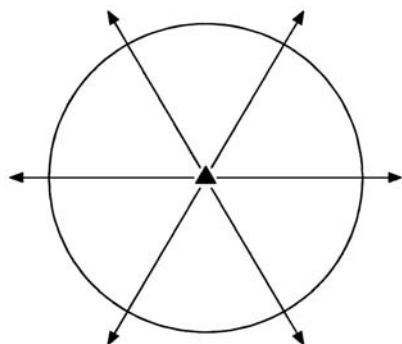
Trigonal

No. 46

$\bar{3}21$

Patterson symmetry $\bar{3}m1$

SECOND SETTING



Origin at 321

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) 2 x,x,0
(2_{xy} 0,0,0) | (5) 2 x,0,0
(2_x 0,0,0) | (6) 2 0,y,0
(2_y 0,0,0) |

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

Positions

Multiplicity, Wyckoff letter, Site symmetry	Coordinates			Reflection conditions
6 <i>f</i> 1	(1) x, y, z (4) y, x, \bar{z}	(2) $\bar{y}, x - y, z$ (5) $x - y, \bar{y}, \bar{z}$	(3) $\bar{x} + y, \bar{x}, z$ (6) $\bar{x}, \bar{x} + y, \bar{z}$	General: no conditions Special: no extra conditions
3 <i>e</i> .2.	$x, 0, \frac{1}{2}$	$0, x, \frac{1}{2}$	$\bar{x}, \bar{x}, \frac{1}{2}$	
3 <i>d</i> .2.	$x, 0, 0$	$0, x, 0$	$\bar{x}, \bar{x}, 0$	
2 <i>c</i> 3..	$0, 0, z$	$0, 0, \bar{z}$		
1 <i>b</i> 32.	$0, 0, \frac{1}{2}$			
1 <i>a</i> 32.	$0, 0, 0$			

Symmetry of special projections

Along [001] $3m$

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

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

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

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

Origin at $0, 0, z$

Origin at $x, 0, 0$

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

IIa none

IIb [3] $\bar{3}_221$ ($\mathbf{c}' = 3\mathbf{c}$) ($\bar{3}_2$, 12, 48); [3] $\bar{3}_121$ ($\mathbf{c}' = 3\mathbf{c}$) ($\bar{3}_1$, 12, 47)

Maximal isotypic subgroups and enantiomorphic subgroups of lowest index

IIc [2] $\bar{3}21$ ($\mathbf{c}' = 2\mathbf{c}$) ($\bar{3}$, 12, 46)

Minimal non-isotypic non-enantiomorphic supergroups

I [2] $\bar{3}1m$ (51); [2] $\bar{3}1c$ (52); [2] $\bar{6}22$ (62); [2] $\bar{6}_322$ (65); [2] $\bar{6}m2$ (71); [2] $\bar{6}c2$ (72)

II none