

$\bar{3}12$

312

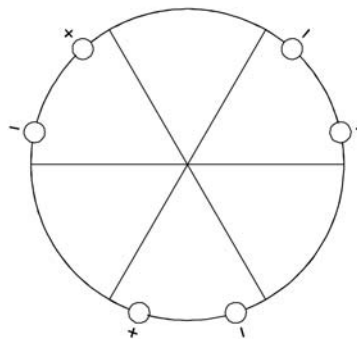
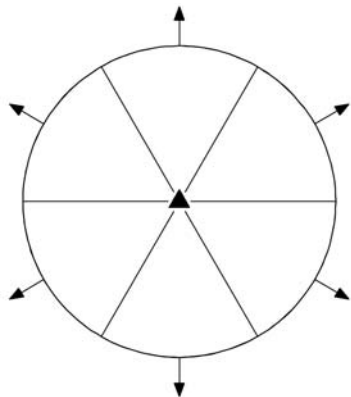
Trigonal

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

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

Positions

		Coordinates			Reflection conditions	
Multiplicity, Wyckoff letter, Site symmetry					General:	
6	f 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	e .. 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	d .. 2	$x, \bar{x}, 0$	$x, 2x, 0$	$2\bar{x}, \bar{x}, 0$		
2	c 3 ..	$0, 0, z$	$0, 0, \bar{z}$			
1	b 3 . 2	$0, 0, \frac{1}{2}$				
1	a 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
	$[3]\bar{1}112$ ($\bar{2}11, 3$)	1; 4
	$[3]\bar{1}112$ ($\bar{2}11, 3$)	1; 5
	$[3]\bar{1}112$ ($\bar{2}11, 3$)	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

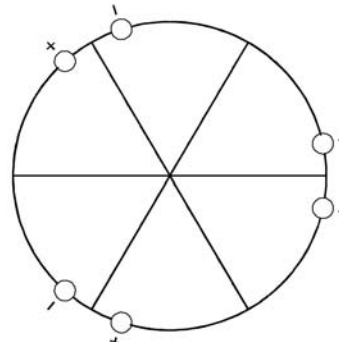
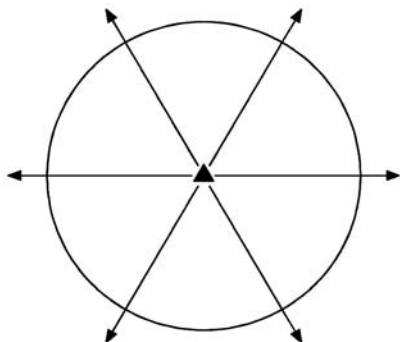
Trigonal

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 | (2) $3^+ 0,0,z$ | (3) $3^- 0,0,z$ |
| (4) 2 $x,x,0$ | (5) 2 $x,0,0$ | (6) 2 $0,y,0$ |

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] $\bar{3}1m1$
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
	$[3]\bar{3}121 (\bar{3}211, 3)$	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	$[3]\bar{3}_221 (\mathbf{c}' = 3\mathbf{c}) (\bar{3}_212, 48)$; $[3]\bar{3}_121 (\mathbf{c}' = 3\mathbf{c}) (\bar{3}_112, 47)$	

Maximal isotypic subgroups and enantiomorphic subgroups of lowest index

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