

$\bar{3}1m$

$\bar{3}1m$

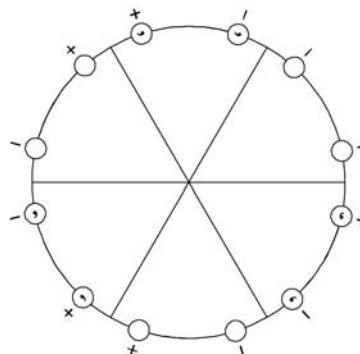
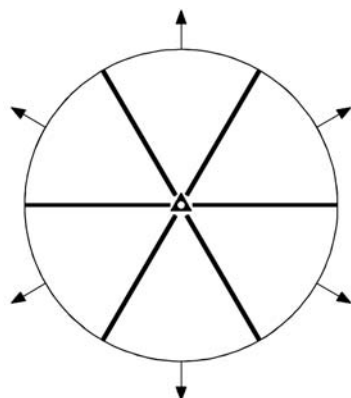
Trigonal

No. 51

$\bar{3}12/m$

Patterson symmetry $\bar{3}1m$

FIRST SETTING



Origin at centre ($\bar{3}1m$)

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

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 $2x, x, 0$ |
| (7) $\bar{1}$ 0,0,0 | (8) $\bar{3}^+$ 0,0,z; 0,0,0 | (9) $\bar{3}^-$ 0,0,z; 0,0,0 |
| (10) m x, x, z | (11) m $x, 0, z$ | (12) m $0, y, z$ |

Generators selected (1); $t(0,0,1)$; (2); (4); (7)

Positions

Multiplicity, Wyckoff letter, Site symmetry	Coordinates							Reflection conditions
12 <i>g</i> 1	(1) x, y, z	(2) $\bar{y}, x - y, z$	(3) $\bar{x} + y, \bar{x}, z$					General: no conditions
	(4) $\bar{y}, \bar{x}, \bar{z}$	(5) $\bar{x} + y, y, \bar{z}$	(6) $x, x - y, \bar{z}$					
	(7) $\bar{x}, \bar{y}, \bar{z}$	(8) $y, \bar{x} + y, \bar{z}$	(9) $x - y, x, \bar{z}$					
	(10) y, x, z	(11) $x - y, \bar{y}, z$	(12) $\bar{x}, \bar{x} + y, z$					Special: no extra conditions
6 <i>f</i> $\dots m$	$x, 0, z$	$0, x, z$	\bar{x}, \bar{x}, z	$0, \bar{x}, \bar{z}$	$\bar{x}, 0, \bar{z}$	x, x, \bar{z}		
6 <i>e</i> $\dots 2$	$x, \bar{x}, \frac{1}{2}$	$x, 2x, \frac{1}{2}$	$2\bar{x}, \bar{x}, \frac{1}{2}$	$\bar{x}, x, \frac{1}{2}$	$\bar{x}, 2\bar{x}, \frac{1}{2}$	$2x, x, \frac{1}{2}$		
6 <i>d</i> $\dots 2$	$x, \bar{x}, 0$	$x, 2x, 0$	$2\bar{x}, \bar{x}, 0$	$\bar{x}, x, 0$	$\bar{x}, 2\bar{x}, 0$	$2x, x, 0$		
2 <i>c</i> $3 \dots m$	$0, 0, z$	$0, 0, \bar{z}$						
1 <i>b</i> $\bar{3} \dots m$	$0, 0, \frac{1}{2}$							
1 <i>a</i> $\bar{3} \dots m$	$0, 0, 0$							

Symmetry of special projections

Along [001] $6mm$

Along [100] $\bar{3}2mm$

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	$[2]\bar{3}1m (\bar{3}1, 49)$	1; 2; 3; 10; 11; 12
	$[2]\bar{3}12 (46)$	1; 2; 3; 4; 5; 6
	$[2]\bar{3}11 (\bar{3}, 45)$	1; 2; 3; 7; 8; 9
	$[3]\bar{1}12/m (\bar{2}/m11, 6)$	1; 4; 7; 10
	$[3]\bar{1}12/m (\bar{2}/m11, 6)$	1; 5; 7; 11
	$[3]\bar{1}12/m (\bar{2}/m11, 6)$	1; 6; 7; 12

IIa none

IIb $[2]\bar{3}1c (c' = 2c) (52)$

Maximal isotypic subgroups and enantiomorphic subgroups of lowest index

IIc $[2]\bar{3}1m (c' = 2c) (51)$

Minimal non-isotypic non-enantiomorphic supergroups

I $[2]\bar{6}/mmm (73); [2]\bar{6}_3/mmc (75)$

II none

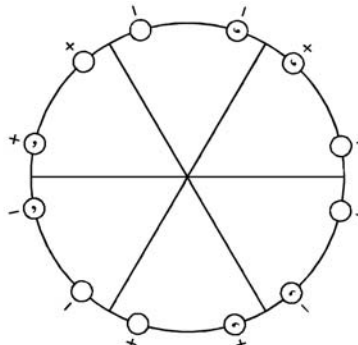
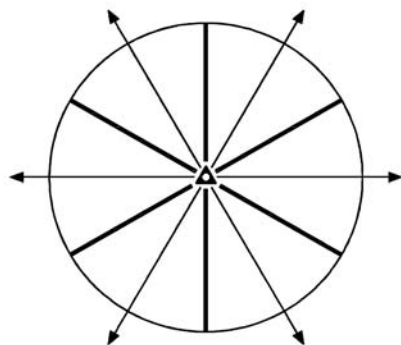
$\bar{3}m1$ $\bar{3}m1$

Trigonal

No. 51

 $\bar{3}2/m1$ Patterson symmetry $\bar{3}m1$

SECOND SETTING

**Origin** at centre ($\bar{3}m1$)**Asymmetric unit** $0 \leq x; 0 \leq y; 0 \leq z \leq 1; y \leq x/2$ **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 |
| (7) $\bar{1}$ 0,0,0 | (8) $\bar{3}^+$ 0,0,z; 0,0,0 | (9) $\bar{3}^-$ 0,0,z; 0,0,0 |
| (10) m x,\bar{x},z | (11) m $x,2x,z$ | (12) m $2x,x,z$ |

Generators selected (1); $t(0,0,1)$; (2); (4); (7)

Positions

Multiplicity, Wyckoff letter, Site symmetry		Coordinates						Reflection conditions
								General:
12 <i>g</i> 1	(1) x, y, z (4) y, x, \bar{z} (7) $\bar{x}, \bar{y}, \bar{z}$ (10) \bar{y}, \bar{x}, z	(2) $\bar{y}, x - y, z$ (5) $x - y, \bar{y}, \bar{z}$ (8) $y, \bar{x} + y, \bar{z}$ (11) $\bar{x} + y, y, z$	(3) $\bar{x} + y, \bar{x}, z$ (6) $\bar{x}, \bar{x} + y, \bar{z}$ (9) $x - y, x, \bar{z}$ (12) $x, x - y, z$					no conditions
								Special: no extra conditions
6 <i>f</i> . <i>m</i> .	x, \bar{x}, z	$x, 2x, z$	$2\bar{x}, \bar{x}, z$	\bar{x}, x, \bar{z}	$2x, x, \bar{z}$	$\bar{x}, 2\bar{x}, \bar{z}$		
6 <i>e</i> .2 .	$x, 0, \frac{1}{2}$	$0, x, \frac{1}{2}$	$\bar{x}, \bar{x}, \frac{1}{2}$	$\bar{x}, 0, \frac{1}{2}$	$0, \bar{x}, \frac{1}{2}$	$x, x, \frac{1}{2}$		
6 <i>d</i> .2 .	$x, 0, 0$	$0, x, 0$	$\bar{x}, \bar{x}, 0$	$\bar{x}, 0, 0$	$0, \bar{x}, 0$	$x, x, 0$		
2 <i>c</i> 3 <i>m</i> .	$0, 0, z$	$0, 0, \bar{z}$						
1 <i>b</i> $\bar{3}m$.	$0, 0, \frac{1}{2}$							
1 <i>a</i> $\bar{3}m$.	$0, 0, 0$							

Symmetry of special projections

Along [001] $6mm$

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

Along [210] $\bar{3}2mm$

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	$[2]\bar{3}m1$ (49)	1; 2; 3; 10; 11; 12
	$[2]\bar{3}21$ ($\bar{3}12, 46$)	1; 2; 3; 4; 5; 6
	$[2]\bar{3}11$ ($\bar{3}, 45$)	1; 2; 3; 7; 8; 9
	$[3]\bar{1}2/m1$ ($\bar{2}/m11, 6$)	1; 4; 7; 10
	$[3]\bar{1}2/m1$ ($\bar{2}/m11, 6$)	1; 5; 7; 11
	$[3]\bar{1}2/m1$ ($\bar{2}/m11, 6$)	1; 6; 7; 12

IIa none

IIb $[2]\bar{3}c1$ ($\mathbf{c}' = 2\mathbf{c}$) ($\bar{3}1c, 52$)

Maximal isotypic subgroups and enantiomorphic subgroups of lowest index

IIc $[2]\bar{3}m1$ ($\mathbf{c}' = 2\mathbf{c}$) ($\bar{3}1m, 51$)

Minimal non-isotypic non-enantiomorphic supergroups

I $[2]\bar{6}/mmm$ (73); $[2]\bar{6}_3/mmc$ (75)

II none