

$\bar{3}m1$

$3m1$

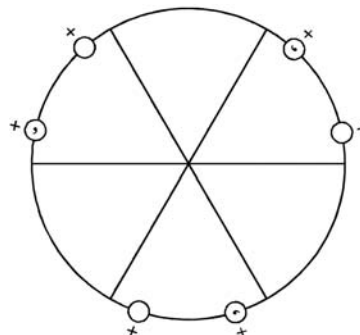
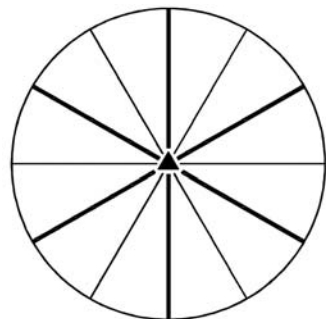
Trigonal

No. 49

$\bar{3}m1$

Patterson symmetry  $\bar{3}m1$

FIRST SETTING



Origin on  $3m1$

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

Symmetry operations

- |   |                                    |   |
|---|------------------------------------|---|
| (1) 1<br>(1 0,0,0)                            | (2) $3^+$ 0,0,z<br>( $3_z$  0,0,0) | (3) $3^-$ 0,0,z<br>( $3_z^{-1}$  0,0,0) |
| (4) $m$ x, $\bar{x}$ ,z<br>( $m_{xy}$  0,0,0) | (5) $m$ x,2x,z<br>( $m_x$  0,0,0)  | (6) $m$ 2x,x,z<br>( $m_y$  0,0,0)       |

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

**Positions**

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

**Symmetry of special projections**

|                     |   |  |
|---------------------|---|--|
| Along [001] $3m$    | Along [100] $\bar{3}1$                            | Along [210] $\bar{3}11m$                                     |
| Origin at $0, 0, z$ | $\mathbf{a}' = \mathbf{c}$<br>Origin at $x, 0, 0$ | $\mathbf{a}' = \mathbf{c}$<br>Origin at $x, \frac{1}{2}x, 0$ |

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

|          |                                    |         |
|----------|------------------------------------|---------|
| <b>I</b> | $[2]\bar{3}11$ ( $\bar{3}, 42$ )   | 1; 2; 3 |
|          | $[3]\bar{1}m1$ ( $\bar{3}m11, 4$ ) | 1; 4    |
|          | $[3]\bar{1}m1$ ( $\bar{3}m11, 4$ ) | 1; 5    |
|          | $[3]\bar{1}m1$ ( $\bar{3}m11, 4$ ) | 1; 6    |

**IIa** none

**IIb**  $[2]\bar{3}c1$  ( $\mathbf{c}' = 2\mathbf{c}$ ) (50)

**Maximal isotypic subgroups and enantiomorphic subgroups of lowest index**

**IIc**  $[2]\bar{3}m1$  ( $\mathbf{c}' = 2\mathbf{c}$ ) (49)

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

**I**  $[2]\bar{3}1m$  (51);  $[2]\bar{6}mm$  (68);  $[2]\bar{6}_3mc$  (70);  $[2]\bar{6}m2$  (71)

**II** none

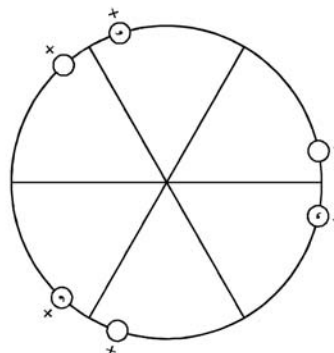
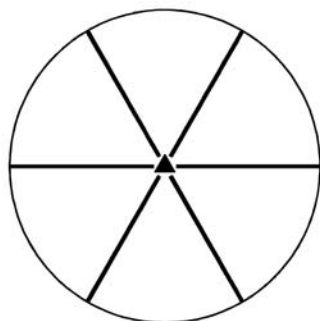
$\bar{3}1m$  $31m$ 

Trigonal

No. 49

 $\bar{3}1m$ Patterson symmetry  $\bar{3}1m$ 

SECOND SETTING

**Origin** on  $31m$ **Asymmetric unit**  $0 \leq x; 0 \leq y; 0 \leq z \leq 1; y \leq x$ **Symmetry operations**

- |                                  |                                    |   |
|----------------------------------|------------------------------------|---|
| (1) 1<br>(1 0,0,0)               | (2) $3^+$ 0,0,z<br>( $3_z$  0,0,0) | (3) $3^-$ 0,0,z<br>( $3_z^{-1}$  0,0,0) |
| (4) $m$ x,x,z<br>( $m_3$  0,0,0) | (5) $m$ x,0,z<br>( $m_2$  0,0,0)   | (6) $m$ 0,y,z<br>( $m_1$  0,0,0)        |

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

**Positions**

|   | Multiplicity,<br>Wyckoff letter,<br>Site symmetry | Coordinates                    |  |  | Reflection conditions   |
|---|---|--------------------------------|--|--|---|
| 6 | $c$ 1   | (1) $x, y, z$<br>(4) $y, x, z$ | (2) $\bar{y}, x - y, z$<br>(5) $x - y, \bar{y}, z$ | (3) $\bar{x} + y, \bar{x}, z$<br>(6) $\bar{x}, \bar{x} + y, z$ | General:<br>no conditions<br><br>Special: no extra conditions |
| 3 | $b$ $\dots m$                                     | $x, 0, z$                      | $0, x, z$  | $\bar{x}, \bar{x}, z$  |   |
| 1 | $a$ $3 \dots m$                                   | $0, 0, z$                      |  |  |   |

**Symmetry of special projections**

|                     |   |  |
|---------------------|---|--|
| Along [001] $3m$    | Along [100] $\bar{3}11m$                          | Along [210] $\bar{3}1$                                       |
| Origin at $0, 0, z$ | $\mathbf{a}' = \mathbf{c}$<br>Origin at $x, 0, 0$ | $\mathbf{a}' = \mathbf{c}$<br>Origin at $x, \frac{1}{2}x, 0$ |

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

|          |                                     |         |
|----------|-------------------------------------|---------|
| <b>I</b> | $[2]\bar{3}111$ ( $\bar{3}3, 42$ )  | 1; 2; 3 |
|          | $[3]\bar{3}11m$ ( $\bar{3}m11, 4$ ) | 1; 4    |
|          | $[3]\bar{3}11m$ ( $\bar{3}m11, 4$ ) | 1; 5    |
|          | $[3]\bar{3}11m$ ( $\bar{3}m11, 4$ ) | 1; 6    |

**IIa** none

**IIb**  $[2]\bar{3}1c$  ( $\mathbf{c}' = 2\mathbf{c}$ ) ( $\bar{3}3c1, 50$ )

**Maximal isotypic subgroups and enantiomorphic subgroups of lowest index**

**IIc**  $[2]\bar{3}1m$  ( $\mathbf{c}' = 2\mathbf{c}$ ) ( $\bar{3}3m1, 49$ )

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

**I**  $[2]\bar{3}\bar{3}1m$  (51);  $[2]\bar{3}6mm$  (68);  $[2]\bar{3}6_3mc$  (70);  $[2]\bar{3}\bar{6}m2$  (71)

**II** none