

$\mu 6_3 m c$

$6 m m$

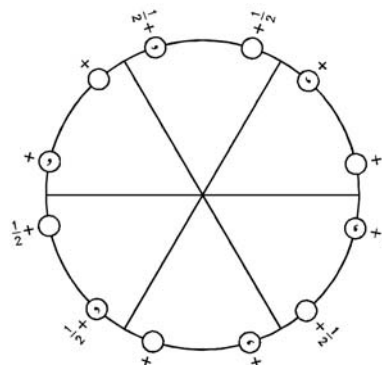
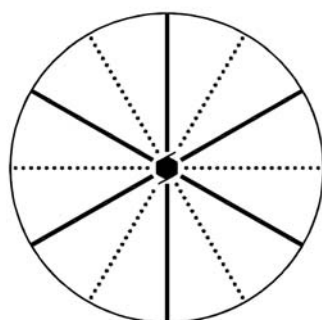
Hexagonal

No. 70

$\mu 6_3 m c$

Patterson symmetry  $\mu 6/m m m$

FIRST SETTING



**Origin** on  $3m1$  on  $6_3mc$

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

**Symmetry operations**

- |   |  |   |
|---|--|---|
| (1) 1<br>(1 0,0,0)  | (2) $3^+ 0,0,z$<br>( $3_2$  0,0,0)                                 | (3) $3^- 0,0,z$<br>( $3_2^{-1}$  0,0,0)                       |
| (4) $2(\frac{1}{2}) 0,0,z$<br>( $2_2$  0,0, $\frac{1}{2}$ ) | (5) $6^-(\frac{1}{2}) 0,0,z$<br>( $6_2^{-1}$  0,0, $\frac{1}{2}$ ) | (6) $6^+(\frac{1}{2}) 0,0,z$<br>( $6_2$  0,0, $\frac{1}{2}$ ) |
| (7) $m x,\bar{x},z$<br>( $m_{xy}$  0,0,0)                   | (8) $m x,2x,z$<br>( $m_x$  0,0,0)                                  | (9) $m 2x,x,z$<br>( $m_y$  0,0,0)                             |
| (10) $c x,x,z$<br>( $m_3$  0,0, $\frac{1}{2}$ )             | (11) $c x,0,z$<br>( $m_2$  0,0, $\frac{1}{2}$ )                    | (12) $c 0,y,z$<br>( $m_1$  0,0, $\frac{1}{2}$ )               |

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

**Positions**

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

**Symmetry of special projections**

Along [001] $6mm$	Along [100] $\mu 11g$	Along [210] $\mu 11m$
Origin at $0, 0, z$	$\mathbf{a}' = \mathbf{c}$ Origin at $x, 0, 0$	$\mathbf{a}' = \frac{1}{2}\mathbf{c}$ Origin at $x, \frac{1}{2}x, 0$

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

<b>I</b>	$[2]\mu 6_3 11 (\mu 6_3, 56)$	1; 2; 3; 4; 5; 6
	$[2]\mu 31c (\mu 3c1, 50)$	1; 2; 3; 10; 11; 12
	$[2]\mu 3m1 (49)$	1; 2; 3; 7; 8; 9
	$[3]\mu 2_1 mc (\mu mc2_1, 17)$	1; 4; 7; 10
	$[3]\mu 2_1 mc (\mu mc2_1, 17)$	1; 4; 8; 11
	$[3]\mu 2_1 mc (\mu mc2_1, 17)$	1; 4; 9; 12

**IIa** none

**IIb** none

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

**IIc**  $[3]\mu 6_3 mc (\mathbf{c}' = 3\mathbf{c}) (70)$

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

**I**  $[2]\mu 6_3 / m m c (75)$

**II**  $[2]\mu 6 m m (\mathbf{c}' = \frac{1}{2}\mathbf{c}) (68)$

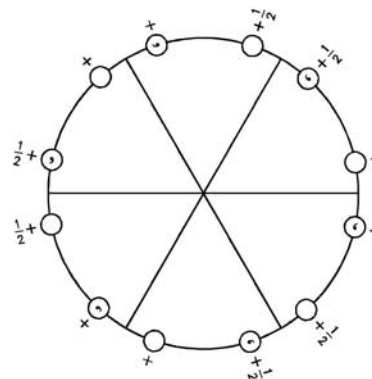
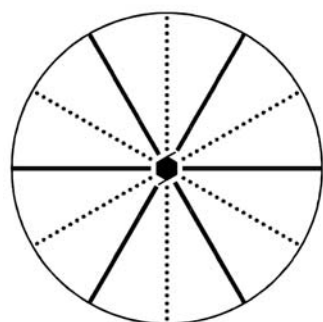
$\mu 6_3 cm$  $6mm$ 

Hexagonal

No. 70

 $\mu 6_3 cm$ Patterson symmetry  $\mu 6/mmm$ 

## SECOND SETTING

**Origin** on  $31m$  on  $6_3cm$ **Asymmetric unit**  $0 \leq x; 0 \leq y; 0 \leq z \leq 1; y \leq x/2$ **Symmetry operations**

- |   |  |   |
|---|--|---|
| (1) 1<br>(1 0,0,0)  | (2) $3^+$ 0,0,z<br>( $3_2$  0,0,0)                                 | (3) $3^-$ 0,0,z<br>( $3_2^{-1}$  0,0,0)                       |
| (4) $2(\frac{1}{2})$ 0,0,z<br>( $2_2$  0,0, $\frac{1}{2}$ ) | (5) $6^-(\frac{1}{2})$ 0,0,z<br>( $6_2^{-1}$  0,0, $\frac{1}{2}$ ) | (6) $6^+(\frac{1}{2})$ 0,0,z<br>( $6_2$  0,0, $\frac{1}{2}$ ) |
| (7) $c$ x, $\bar{x}$ ,z<br>( $m_{xy}$  0,0, $\frac{1}{2}$ ) | (8) $c$ x,2x,z<br>( $m_x$  0,0, $\frac{1}{2}$ )                    | (9) $c$ 2x,x,z<br>( $m_y$  0,0, $\frac{1}{2}$ )               |
| (10) $m$ x,x,z<br>( $m_3$  0,0,0)                           | (11) $m$ x,0,z<br>( $m_2$  0,0,0)                                  | (12) $m$ 0,y,z<br>( $m_1$  0,0,0)                             |

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

**Positions**

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

**Symmetry of special projections**

Along [001]  $6mm$

Along [100]  $\mu 11m$

Along [210]  $\mu 11g$

Origin at  $0, 0, z$

$\mathbf{a}' = \frac{1}{2}\mathbf{c}$

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

Origin at  $x, 0, 0$

Origin at  $x, \frac{1}{2}x, 0$

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

<b>I</b>	$[2] \mu 6_3 11 (\mu 6_3, 56)$	1; 2; 3; 4; 5; 6
	$[2] \mu 3c1 (50)$	1; 2; 3; 7; 8; 9
	$[2] \mu 31m (\mu 3m1, 49)$	1; 2; 3; 10; 11; 12
	$[3] \mu 2_1 cm (\mu mc2_1, 17)$	1; 4; 7; 10
	$[3] \mu 2_1 cm (\mu mc2_1, 17)$	1; 4; 8; 11
	$[3] \mu 2_1 cm (\mu mc2_1, 17)$	1; 4; 9; 12

**IIa** none

**IIb** none

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

**IIc**  $[3] \mu 6_3 cm (\mathbf{c}' = 3\mathbf{c}) (\mu 6_3 mc, 70)$

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

**I**  $[2] \mu 6_3 / m m c (75)$

**II**  $[2] \mu 6 m m (\mathbf{c}' = \frac{1}{2}\mathbf{c}) (68)$