

$\bar{6}m2$

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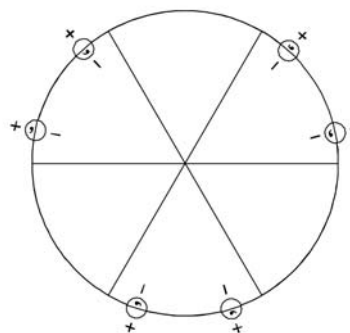
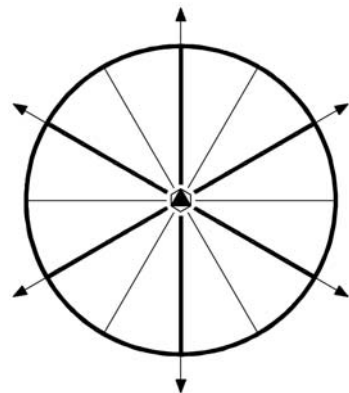
Hexagonal

No. 71

$\bar{6}m2$

Patterson symmetry  $\bar{6}/mmm$

FIRST SETTING



Origin on  $\bar{6}m2$

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

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,y,0<br>( $m_z$  0,0,0)              | (5) $\bar{6}^-$ 0,0,z; 0,0,0<br>( $\bar{6}_z^{-1}$  0,0,0) | (6) $\bar{6}^+$ 0,0,z; 0,0,0<br>( $\bar{6}_z$  0,0,0) |
| (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) 2 x, $\bar{x}$ ,0<br>( $2_3$  0,0,0)     | (11) 2 x,2x,0<br>( $2_2$  0,0,0)                           | (12) 2 2x,x,0<br>( $2_1$  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>i</i> 1	(1) $x, y, z$ (4) $x, y, \bar{z}$ (7) $\bar{y}, \bar{x}, z$ (10) $\bar{y}, \bar{x}, \bar{z}$	(2) $\bar{y}, x - y, z$ (5) $\bar{y}, x - y, \bar{z}$ (8) $\bar{x} + y, y, z$ (11) $\bar{x} + y, y, \bar{z}$	(3) $\bar{x} + y, \bar{x}, z$ (6) $\bar{x} + y, \bar{x}, \bar{z}$ (9) $x, x - y, z$ (12) $x, x - y, \bar{z}$	no conditions		
					Special: no extra conditions		
6	<i>h</i> . <i>m</i> .	$x, \bar{x}, z$	$x, 2x, z$	$2\bar{x}, \bar{x}, z$	$x, \bar{x}, \bar{z}$	$x, 2x, \bar{z}$	$2\bar{x}, \bar{x}, \bar{z}$
6	<i>g</i> <i>m</i> . .	$x, y, \frac{1}{2}$	$\bar{y}, x - y, \frac{1}{2}$	$\bar{x} + y, \bar{x}, \frac{1}{2}$	$\bar{y}, \bar{x}, \frac{1}{2}$	$\bar{x} + y, y, \frac{1}{2}$	$x, x - y, \frac{1}{2}$
6	<i>f</i> <i>m</i> . .	$x, y, 0$	$\bar{y}, x - y, 0$	$\bar{x} + y, \bar{x}, 0$	$\bar{y}, \bar{x}, 0$	$\bar{x} + y, y, 0$	$x, x - y, 0$
3	<i>e</i> <i>m m</i> 2	$x, \bar{x}, \frac{1}{2}$	$x, 2x, \frac{1}{2}$	$2\bar{x}, \bar{x}, \frac{1}{2}$			
3	<i>d</i> <i>m m</i> 2	$x, \bar{x}, 0$	$x, 2x, 0$	$2\bar{x}, \bar{x}, 0$			
2	<i>c</i> 3 <i>m</i> .	$0, 0, z$	$0, 0, \bar{z}$				
1	<i>b</i> $\bar{6}m2$	$0, 0, \frac{1}{2}$					
1	<i>a</i> $\bar{6}m2$	$0, 0, 0$					

**Symmetry of special projections**

Along [001] 3*m*

Along [100]  $\bar{6}m2$

Along [210]  $\bar{6}m2$

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

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

Origin at 0, 0, *z*

Origin at  $x, 0, 0$

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

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

<b>I</b>	[2] $\bar{6}11$ ( $\bar{6}$ , 59)	1; 2; 3; 4; 5; 6
	[2] $\bar{3}m1$ (49)	1; 2; 3; 7; 8; 9
	[2] $\bar{3}12$ (46)	1; 2; 3; 10; 11; 12
	[3] $\bar{2}m2$ ( $\bar{2}mm$ , 18)	1; 4; 7; 10
	[3] $\bar{2}m2$ ( $\bar{2}mm$ , 18)	1; 4; 8; 11
	[3] $\bar{2}m2$ ( $\bar{2}mm$ , 18)	1; 4; 9; 12

**IIa** none

**IIb** [2]  $\bar{6}c2$  ( $\mathbf{c}' = 2\mathbf{c}$ ) (72)

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

**IIc** [2]  $\bar{6}m2$  ( $\mathbf{c}' = 2\mathbf{c}$ ) (71)

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

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

**II** none

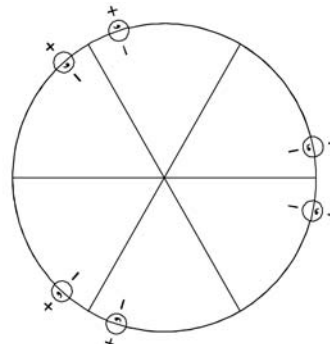
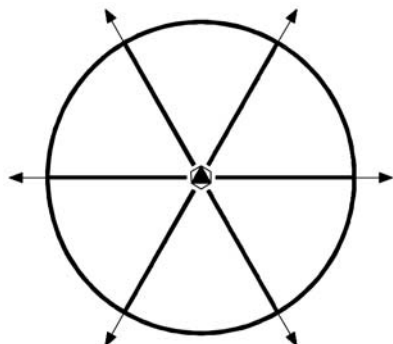
$\bar{6}2m$  $\bar{6}2m$ 

Hexagonal

No. 71

 $\bar{6}2m$ Patterson symmetry  $\bar{6}/mmm$ 

## SECOND SETTING

**Origin** on  $\bar{6}2m$ **Asymmetric unit**  $0 \leq x; 0 \leq y; 0 \leq z \leq \frac{1}{2}; y \leq x$ **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>( $3_z^+$  0,0,0)                    |
| (4) $m$ x,y,0<br>( $m_z$  0,0,0)  | (5) $\bar{6}^-$ 0,0,z; 0,0,0<br>( $\bar{6}_z^-$  0,0,0) | (6) $\bar{6}^+$ 0,0,z; 0,0,0<br>( $\bar{6}_z^+$  0,0,0) |
| (7) 2 x,x,0<br>( $2_{xy}$  0,0,0) | (8) 2 x,0,0<br>( $2_x$  0,0,0)                          | (9) 2 0,y,0<br>( $2_y$  0,0,0)                          |
| (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>i</i>	1	(1) $x, y, z$ (4) $x, y, \bar{z}$ (7) $y, x, \bar{z}$ (10) $y, x, z$	(2) $\bar{y}, x - y, z$ (5) $\bar{y}, x - y, \bar{z}$ (8) $x - y, \bar{y}, \bar{z}$ (11) $x - y, \bar{y}, z$	(3) $\bar{x} + y, \bar{x}, z$ (6) $\bar{x} + y, \bar{x}, \bar{z}$ (9) $\bar{x}, \bar{x} + y, \bar{z}$ (12) $\bar{x}, \bar{x} + y, z$	no conditions		
Special: no extra conditions								
6	<i>h</i>	$m \dots$	$x, y, \frac{1}{2}$	$\bar{y}, x - y, \frac{1}{2}$	$\bar{x} + y, \bar{x}, \frac{1}{2}$	$y, x, \frac{1}{2}$	$x - y, \bar{y}, \frac{1}{2}$	$\bar{x}, \bar{x} + y, \frac{1}{2}$
6	<i>g</i>	$m \dots$	$x, y, 0$	$\bar{y}, x - y, 0$	$\bar{x} + y, \bar{x}, 0$	$y, x, 0$	$x - y, \bar{y}, 0$	$\bar{x}, \bar{x} + y, 0$
6	<i>f</i>	$\dots m$	$x, 0, z$	$0, x, z$	$\bar{x}, \bar{x}, z$	$x, 0, \bar{z}$	$0, x, \bar{z}$	$\bar{x}, \bar{x}, \bar{z}$
3	<i>e</i>	$m 2 m$	$x, 0, \frac{1}{2}$	$0, x, \frac{1}{2}$	$\bar{x}, \bar{x}, \frac{1}{2}$			
3	<i>d</i>	$m 2 m$	$x, 0, 0$	$0, x, 0$	$\bar{x}, \bar{x}, 0$			
2	<i>c</i>	$3 \dots m$	$0, 0, z$	$0, 0, \bar{z}$				
1	<i>b</i>	$\bar{6} 2 m$	$0, 0, \frac{1}{2}$					
1	<i>a</i>	$\bar{6} 2 m$	$0, 0, 0$					

**Symmetry of special projections**

Along [001] $3m$	Along [100] $\bar{6}2m$ $\mathbf{a}' = \mathbf{c}$ Origin at $x, 0, 0$	Along [210] $\bar{6}1m1$ $\mathbf{a}' = \mathbf{c}$ Origin at $x, \frac{1}{2}x, 0$
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**Maximal non-isotypic non-enantiomorphic subgroups**

<b>I</b>	$[2]\bar{6}11 (\bar{6}, 59)$	1; 2; 3; 4; 5; 6
	$[2]\bar{6}31m (\bar{6}3m1, 49)$	1; 2; 3; 10; 11; 12
	$[2]\bar{6}321 (\bar{6}312, 46)$	1; 2; 3; 7; 8; 9
	$[3]\bar{6}m2m (\bar{6}2mm, 18)$	1; 4; 7; 10
	$[3]\bar{6}m2m (\bar{6}2mm, 18)$	1; 4; 8; 11
	$[3]\bar{6}m2m (\bar{6}2mm, 18)$	1; 4; 9; 12

**IIa** none

**IIb**  $[2]\bar{6}2c (\mathbf{c}' = 2\mathbf{c}) (\bar{6}2c, 72)$

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

**IIc**  $[2]\bar{6}2m (\mathbf{c}' = 2\mathbf{c}) (\bar{6}2m, 71)$

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

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

**II** none