

$\mu 6_3/mmc$

$6/mmm$

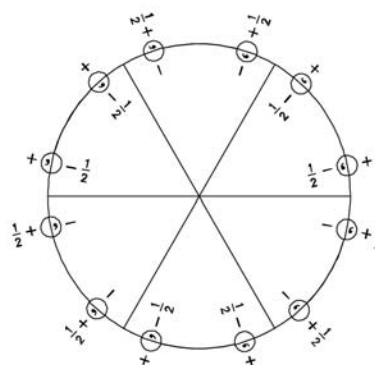
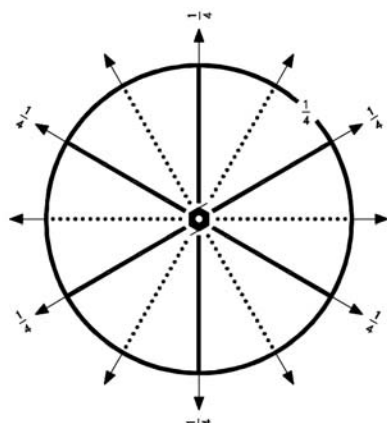
Hexagonal

No. 75

$\mu 6_3/m2/m2/c$

Patterson symmetry $\mu 6/mmm$

FIRST SETTING



Origin at centre ($\bar{3}m1$) at $\bar{3}2/mc$

Asymmetric unit $y \leq x/2; -x \leq y; 0 \leq z \leq \frac{1}{4}$

Symmetry operations

- | | | |
|---|--|--|
| (1) 1
(1 0,0,0) | (2) $3^+ 0,0,z$
(3_2^+ 0,0,0) | (3) $3^- 0,0,z$
(3_2^- 0,0,0) |
| (4) $2(\frac{1}{2}) 0,0,z$
(2_2 0,0, $\frac{1}{2}$) | (5) $6^-(\frac{1}{2}) 0,0,z$
(6_2^- 0,0, $\frac{1}{2}$) | (6) $6^+(\frac{1}{2}) 0,0,z$
(6_2^+ 0,0, $\frac{1}{2}$) |
| (7) 2 $x,x,0$
(2_{xy} 0,0,0) | (8) 2 $x,0,0$
(2_x 0,0,0) | (9) 2 $0,y,0$
(2_y 0,0,0) |
| (10) 2 $x,\bar{x},\frac{1}{4}$
(2_3 0,0, $\frac{1}{2}$) | (11) 2 $x,2x,\frac{1}{4}$
(2_2 0,0, $\frac{1}{2}$) | (12) 2 $2x,x,\frac{1}{4}$
(2_1 0,0, $\frac{1}{2}$) |
| (13) $\bar{1} 0,0,0$
($\bar{1}$ 0,0,0) | (14) $\bar{3}^+ 0,0,z; 0,0,0$
($\bar{3}_2^+$ 0,0,0) | (15) $\bar{3}^- 0,0,z; 0,0,0$
($\bar{3}_2^-$ 0,0,0) |
| (16) $m x,y,\frac{1}{4}$
(m_z 0,0, $\frac{1}{2}$) | (17) $\bar{6}^- 0,0,z; 0,0,\frac{1}{4}$
($\bar{6}_2^-$ 0,0, $\frac{1}{2}$) | (18) $\bar{6}^+ 0,0,z; 0,0,\frac{1}{4}$
($\bar{6}_2^+$ 0,0, $\frac{1}{2}$) |
| (19) $m x,\bar{x},z$
(m_{xy} 0,0,0) | (20) $m x,2x,z$
(m_x 0,0,0) | (21) $m 2x,x,z$
(m_y 0,0,0) |
| (22) $c x,x,z$
(m_3 0,0, $\frac{1}{2}$) | (23) $c x,0,z$
(m_2 0,0, $\frac{1}{2}$) | (24) $c 0,y,z$
(m_1 0,0, $\frac{1}{2}$) |

Generators selected (1); $t(0,0,1)$; (2); (4); (7); (13)

Positions

Multiplicity, Wyckoff letter, Site symmetry	Coordinates	Reflection conditions
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					General:
24	$h\ 1$	(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) y, x, \bar{z}	(8) $x - y, \bar{y}, \bar{z}$	(9) $\bar{x}, \bar{x} + y, \bar{z}$	
		(10) $\bar{y}, \bar{x}, \bar{z} + \frac{1}{2}$	(11) $\bar{x} + y, y, \bar{z} + \frac{1}{2}$	(12) $x, x - y, \bar{z} + \frac{1}{2}$	
		(13) $\bar{x}, \bar{y}, \bar{z}$	(14) $y, \bar{x} + y, \bar{z}$	(15) $x - y, x, \bar{z}$	
		(16) $x, y, \bar{z} + \frac{1}{2}$	(17) $\bar{y}, x - y, \bar{z} + \frac{1}{2}$	(18) $\bar{x} + y, \bar{x}, \bar{z} + \frac{1}{2}$	
		(19) \bar{y}, \bar{x}, z	(20) $\bar{x} + y, y, z$	(21) $x, x - y, z$	
		(22) $y, x, z + \frac{1}{2}$	(23) $x - y, \bar{y}, z + \frac{1}{2}$	(24) $\bar{x}, \bar{x} + y, z + \frac{1}{2}$	

Special: no extra conditions

12	$g\ .m.$	$x, 2x, z$ $2x, x, \bar{z}$	$2\bar{x}, \bar{x}, z$ $\bar{x}, 2\bar{x}, \bar{z}$	x, \bar{x}, z \bar{x}, x, \bar{z}	$\bar{x}, 2\bar{x}, z + \frac{1}{2}$ $2\bar{x}, \bar{x}, \bar{z} + \frac{1}{2}$	$2x, x, z + \frac{1}{2}$ $x, 2x, \bar{z} + \frac{1}{2}$	$\bar{x}, x, z + \frac{1}{2}$ $x, \bar{x}, \bar{z} + \frac{1}{2}$
12	$f\ m..$	$x, y, \frac{1}{4}$ $y, x, \frac{3}{4}$	$\bar{y}, x - y, \frac{1}{4}$ $x - y, \bar{y}, \frac{3}{4}$	$\bar{x} + y, \bar{x}, \frac{1}{4}$ $\bar{x}, \bar{x} + y, \frac{3}{4}$	$\bar{x}, \bar{y}, \frac{3}{4}$ $\bar{y}, \bar{x}, \frac{1}{4}$	$y, \bar{x} + y, \frac{3}{4}$ $\bar{x} + y, y, \frac{1}{4}$	$x - y, x, \frac{3}{4}$ $x, x - y, \frac{1}{4}$
12	$e\ .2.$	$x, 0, 0$ $\bar{x}, 0, 0$	$0, x, 0$ $0, \bar{x}, 0$	$\bar{x}, \bar{x}, 0$ $x, x, 0$	$\bar{x}, 0, \frac{1}{2}$ $x, 0, \frac{1}{2}$	$0, \bar{x}, \frac{1}{2}$ $0, x, \frac{1}{2}$	$x, x, \frac{1}{2}$ $\bar{x}, \bar{x}, \frac{1}{2}$
6	$d\ mm2$	$x, 2x, \frac{1}{4}$	$2\bar{x}, \bar{x}, \frac{1}{4}$	$x, \bar{x}, \frac{1}{4}$	$\bar{x}, 2\bar{x}, \frac{3}{4}$	$2x, x, \frac{3}{4}$	$\bar{x}, x, \frac{3}{4}$
4	$c\ 3m.$	$0, 0, z$	$0, 0, z + \frac{1}{2}$	$0, 0, \bar{z}$	$0, 0, \bar{z} + \frac{1}{2}$		
2	$b\ \bar{6}m2$	$0, 0, \frac{1}{4}$	$0, 0, \frac{3}{4}$				
2	$a\ \bar{3}m.$	$0, 0, 0$	$0, 0, \frac{1}{2}$				

Symmetry of special projections

Along [001] $6mm$

Along [100] $\bar{6}2mg$

Along [210] $\bar{6}2mm$

Origin at $0, 0, z$

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

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

Origin at $x, 0, 0$

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

Maximal non-isotypic non-enantiomorphic subgroups

I	$[2]\bar{6}2c (\bar{6}2c2, 72)$	1; 2; 3; 7; 8; 9; 16; 17; 18; 22; 23; 24
	$[2]\bar{6}m2 (71)$	1; 2; 3; 10; 11; 12; 16; 17; 18; 19; 20; 21
	$[2]\bar{6}_3mc (70)$	1; 2; 3; 4; 5; 6; 19; 20; 21; 22; 23; 24
	$[2]\bar{6}_322 (65)$	1; 2; 3; 4; 5; 6; 7; 8; 9; 10; 11; 12
	$[2]\bar{6}_3/m11 (\bar{6}_3/m, 61)$	1; 2; 3; 4; 5; 6; 13; 14; 15; 16; 17; 18
	$[2]\bar{3}1c (52)$	1; 2; 3; 10; 11; 12; 13; 14; 15; 22; 23; 24
	$[2]\bar{3}m1 (\bar{3}1m, 51)$	1; 2; 3; 7; 8; 9; 13; 14; 15; 19; 20; 21
	$[3]\bar{6}mmc (\bar{6}mcm, 22)$	1; 4; 7; 10; 13; 16; 19; 22
	$[3]\bar{6}mmc (\bar{6}mcm, 22)$	1; 4; 8; 11; 13; 16; 20; 23
	$[3]\bar{6}mmc (\bar{6}mcm, 22)$	1; 4; 9; 12; 13; 16; 21; 24

IIa none

IIb none

Maximal isotypic subgroups and enantiomorphic subgroups of lowest index

IIc $[3]\bar{6}_3/mmc (\mathbf{c}' = 3\mathbf{c}) (75)$

Minimal non-isotypic non-enantiomorphic supergroups

I none

II $[2]\bar{6}/mmm (\mathbf{c}' = \frac{1}{2}\mathbf{c}) (73)$

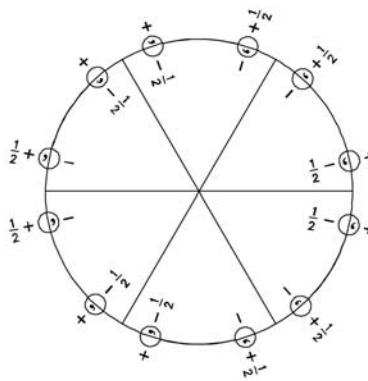
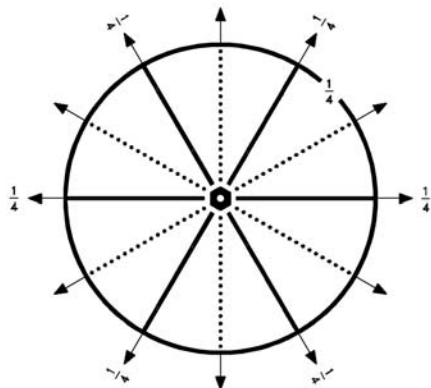
$\mu 6_3/mcm$ $6/mmm$

Hexagonal

No. 75

 $\mu 6_3/m2/c2/m$ Patterson symmetry $\mu 6/mmm$

SECOND SETTING

Origin at centre ($\bar{3}1m$) at $\bar{3}c2/m$ Asymmetric unit $0 \leq x$; $0 \leq y$; $0 \leq z \leq \frac{1}{4}$; $y \leq x$

Symmetry operations

- | | | |
|--|--|---|
| (1) 1
(1 0,0,0) | (2) 3^+ 0,0,z
(3_2 0,0,0) | (3) 3^- 0,0,z
(3_2^{-1} 0,0,0) |
| (4) $2(\frac{1}{2})$ 0,0,z
(2_2 0,0, $\frac{1}{2}$) | (5) $6^-(\frac{1}{2})$ 0,0,z
(6_2^{-1} 0,0, $\frac{1}{2}$) | (6) $6^+(\frac{1}{2})$ 0,0,z
(6_2 0,0, $\frac{1}{2}$) |
| (7) 2 x,x, $\frac{1}{4}$
(2_{xy} 0,0, $\frac{1}{2}$) | (8) 2 x,0, $\frac{1}{4}$
(2_x 0,0, $\frac{1}{2}$) | (9) 2 0,y, $\frac{1}{4}$
(2_y 0,0, $\frac{1}{2}$) |
| (10) 2 x, \bar{x} ,0
(2_3 0,0,0) | (11) 2 x,2x,0
(2_2 0,0,0) | (12) 2 2x,x,0
(2_1 0,0,0) |
| (13) $\bar{1}$ 0,0,0
($\bar{1}$ 0,0,0) | (14) $\bar{3}^+$ 0,0,z; 0,0,0
($\bar{3}_2$ 0,0,0) | (15) $\bar{3}^-$ 0,0,z; 0,0,0
($\bar{3}_2^{-1}$ 0,0,0) |
| (16) m x,y, $\frac{1}{4}$
(m_z 0,0, $\frac{1}{2}$) | (17) $\bar{6}^-$ 0,0,z; 0,0, $\frac{1}{4}$
($\bar{6}_2^{-1}$ 0,0, $\frac{1}{2}$) | (18) $\bar{6}^+$ 0,0,z; 0,0, $\frac{1}{4}$
($\bar{6}_2$ 0,0, $\frac{1}{2}$) |
| (19) c x, \bar{x} ,z
(m_{xy} 0,0, $\frac{1}{2}$) | (20) c x,2x,z
(m_x 0,0, $\frac{1}{2}$) | (21) c 2x,x,z
(m_y 0,0, $\frac{1}{2}$) |
| (22) m x,x,z
(m_3 0,0,0) | (23) m x,0,z
(m_2 0,0,0) | (24) m 0,y,z
(m_1 0,0,0) |

Generators selected (1); $t(0,0,1)$; (2); (4); (7); (13)

Positions

Multiplicity, Wyckoff letter, Site symmetry		Coordinates						Reflection conditions		
								General:		
24	<i>h</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) $y, x, \bar{z} + \frac{1}{2}$	(8) $x - y, \bar{y}, \bar{z} + \frac{1}{2}$	(9) $\bar{x}, \bar{x} + y, \bar{z} + \frac{1}{2}$						
		(10) $\bar{y}, \bar{x}, \bar{z}$	(11) $\bar{x} + y, y, \bar{z}$	(12) $x, x - y, \bar{z}$						
		(13) $\bar{x}, \bar{y}, \bar{z}$	(14) $y, \bar{x} + y, \bar{z}$	(15) $x - y, x, \bar{z}$						
		(16) $x, y, \bar{z} + \frac{1}{2}$	(17) $\bar{y}, x - y, \bar{z} + \frac{1}{2}$	(18) $\bar{x} + y, \bar{x}, \bar{z} + \frac{1}{2}$						
		(19) $\bar{y}, \bar{x}, z + \frac{1}{2}$	(20) $\bar{x} + y, y, z + \frac{1}{2}$	(21) $x, x - y, z + \frac{1}{2}$						
		(22) y, x, z	(23) $x - y, \bar{y}, z$	(24) $\bar{x}, \bar{x} + y, z$						
		Special: no extra conditions								
		12	<i>g</i> $\dots m$	$x, 0, z$	$0, x, z$	\bar{x}, \bar{x}, z	$\bar{x}, 0, z + \frac{1}{2}$		$0, \bar{x}, z + \frac{1}{2}$	$x, x, z + \frac{1}{2}$
				$0, x, \bar{z} + \frac{1}{2}$	$x, 0, \bar{z} + \frac{1}{2}$	$\bar{x}, \bar{x}, \bar{z} + \frac{1}{2}$	$0, \bar{x}, \bar{z}$		$\bar{x}, 0, \bar{z}$	x, x, \bar{z}
		12	<i>f</i> $m \dots$	$x, y, \frac{1}{4}$	$\bar{y}, x - y, \frac{1}{4}$	$\bar{x} + y, \bar{x}, \frac{1}{4}$	$\bar{x}, \bar{y}, \frac{3}{4}$		$y, \bar{x} + y, \frac{3}{4}$	$x - y, x, \frac{3}{4}$
				$y, x, \frac{1}{4}$	$x - y, \bar{y}, \frac{1}{4}$	$\bar{x}, \bar{x} + y, \frac{1}{4}$	$\bar{y}, \bar{x}, \frac{3}{4}$		$\bar{x} + y, y, \frac{3}{4}$	$x, x - y, \frac{3}{4}$
		12	<i>e</i> $\dots 2$	$x, 2x, 0$	$2\bar{x}, \bar{x}, 0$	$x, \bar{x}, 0$	$\bar{x}, 2\bar{x}, \frac{1}{2}$		$2x, x, \frac{1}{2}$	$\bar{x}, x, \frac{1}{2}$
				$\bar{x}, 2\bar{x}, 0$	$2x, x, 0$	$\bar{x}, x, 0$	$x, 2x, \frac{1}{2}$		$2\bar{x}, \bar{x}, \frac{1}{2}$	$x, \bar{x}, \frac{1}{2}$
		6	<i>d</i> $m 2 m$	$x, 0, \frac{1}{4}$	$0, x, \frac{1}{4}$	$\bar{x}, \bar{x}, \frac{1}{4}$	$\bar{x}, 0, \frac{3}{4}$		$0, \bar{x}, \frac{3}{4}$	$x, x, \frac{3}{4}$
		4	<i>c</i> $3 \dots m$	$0, 0, z$	$0, 0, z + \frac{1}{2}$	$0, 0, \bar{z} + \frac{1}{2}$	$0, 0, \bar{z}$			
		2	<i>b</i> $\bar{3} \dots m$	$0, 0, 0$	$0, 0, \frac{1}{2}$					
		2	<i>a</i> $\bar{6} 2 m$	$0, 0, \frac{1}{4}$	$0, 0, \frac{3}{4}$					

Symmetry of special projections

Along [001] $6mm$

Along [100] $\mu 2mm$

Along [210] $\mu 2mg$

Origin at $0, 0, z$

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

Origin at $x, 0, 0$

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

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

Maximal non-isotypic non-enantiomorphic subgroups

I	$[2]\mu\bar{6}c2$ (72)	1; 2; 3; 10; 11; 12; 16; 17; 18; 19; 20; 21
	$[2]\mu\bar{6}2m$ ($\mu\bar{6}m2$, 71)	1; 2; 3; 7; 8; 9; 16; 17; 18; 22; 23; 24
	$[2]\mu 6_3 cm$ ($\mu 6_3 mc$, 70)	1; 2; 3; 4; 5; 6; 19; 20; 21; 22; 23; 24
	$[2]\mu 6_3 22$ (65)	1; 2; 3; 4; 5; 6; 7; 8; 9; 10; 11; 12
	$[2]\mu 6_3/m 11$ ($\mu 6_3/m$, 61)	1; 2; 3; 4; 5; 6; 13; 14; 15; 16; 17; 18
	$[2]\mu\bar{3}c1$ ($\mu\bar{3}1c$, 52)	1; 2; 3; 7; 8; 9; 13; 14; 15; 19; 20; 21
	$[2]\mu\bar{3}1m$ (51)	1; 2; 3; 10; 11; 12; 13; 14; 15; 22; 23; 24
	$[3]\mu mcm$ (μmcm , 22)	1; 4; 7; 10; 13; 16; 19; 22
	$[3]\mu mcm$ (μmcm , 22)	1; 4; 8; 11; 13; 16; 20; 23
	$[3]\mu mcm$ (μmcm , 22)	1; 4; 9; 12; 13; 16; 21; 24

IIa none

IIb none

Maximal isotypic subgroups and enantiomorphic subgroups of lowest index

IIc $[3]\mu 6_3/mcm$ ($\mathbf{c}' = 3\mathbf{c}$) ($\mu 6_3/mmc$, 75)

Minimal non-isotypic non-enantiomorphic supergroups

I none

II $[2]\mu 6/mmm$ ($\mathbf{c}' = \frac{1}{2}\mathbf{c}$) (73)